P-PROPYLBENZOIC ACID

Other names:	4-propylbenzoic acid
	benzoic acid, 4-propyl-
	p-n-Propyl benzoic acid
Inchi:	InChI=1S/C10H12O2/c1-2-3-8-4-6-9(7-5-8)10(11)12/h4-7H,2-3H2,1H3,(H,11,12)
InchiKey:	ATZHGRNFEFVDDJ-UHFFFAOYSA-N
Formula:	C10H12O2
SMILES:	CCCc1ccc(C(=O)O)cc1
Mol. weight [g/mol]:	164.20
CAS:	2438-05-3

Physical Properties

Property code	Value	Unit	Source
af	0.7385		Cheméo Relay (1.0)
gf	-129.64	kJ/mol	Joback Method
hf	-367.83	kJ/mol	Cheméo Relay (1.0)
hfus	19.67	kJ/mol	Thermodynamic study of the sublimation of eight 4-n-alkylbenzoic acids
hsub	109.10 ± 0.80	kJ/mol	NIST Webbook
hvap	91.60	kJ/mol	Cheméo Relay (1.0)
ie	9.30	eV	Cheméo Relay (1.0)
log10ws	-3.20		Cheméo Relay (1.0)
logp	2.337		Crippen Method
mcvol	135.440	ml/mol	McGowan Method
pc	3431.89	kPa	Joback Method
tb	556.42	K	Cheméo Relay (1.0)
tc	768.97	K	Cheméo Relay (1.0)
tf	422.00 ± 0.20	K	NIST Webbook
vc	0.486	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	326.71	J/mol×K	605.91	Joback Method

cpg	337.80	J/mol×K	639.45	Joback Method
cpg	348.25	J/mol×K	672.98	Joback Method
cpg	358.07	J/mol×K	706.52	Joback Method
cpg	367.30	J/mol×K	740.05	Joback Method
cpg	375.96	J/mol×K	773.59	Joback Method
cpg	384.07	J/mol×K	807.12	Joback Method
dvisc	0.0039982	Pa×s	352.15	Joback Method
dvisc	0.0015091	Pa×s	394.44	Joback Method
dvisc	0.0006879	Pa×s	436.74	Joback Method
dvisc	0.0003602	Pa×s	479.03	Joback Method
dvisc	0.0002095	Pa×s	521.32	Joback Method
dvisc	0.0001322	Pa×s	563.62	Joback Method
dvisc	0.0000889	Pa×s	605.91	Joback Method
hfust	23.30	kJ/mol	422.00	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.37953e+01
Coeff. B	-4.34318e+03
Coeff. C	-8.84900e+01
Temperature range (K), min.	410.02
Temperature range (K), max.	600.43

Sources

Thermodynamic study of the sublimation of eight 4-n-alkylbenzoic acids:	https://www.doi.org/10.1016/j.jct.2004.02.001
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2438053&Units=SI
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0, beta):	
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Cheméo Relay (1.0):	

Legend

af:	Acentric Factor
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
pvap:	Vapor pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume