BENZOIC ACID, 4-HEPTYL-

Other names: 4-heptylbenzoic acid
p-heptylbenzoic acid
Inchi: InChI=1S/C14H20O2/c1-2-3-4-5-6-7-12-8-10-13(11-9-12)14(15)16/h8-11H,2-7H2,1H3,(H
InchiKey: VSUKEWPHURLYTK-UHFFFAOYSA-N
Formula: C14H20O2
SMILES: CCCCCCCc1ccc(C(=O)O)cc1
Mol. weight [g/mol]: 220.31
CAS: 38350-87-7

Physical Properties

Property code	Value	Unit	Source
af	0.8953		Cheméo Relay (1.0)
gf	-95.96	kJ/mol	Joback Method
hf	-452.06	kJ/mol	Cheméo Relay (1.0)
hfus	1.00	kJ/mol	Thermodynamic study of the sublimation of eight 4-n-alkylbenzoic acids
hsub	130.00 ± 0.90	kJ/mol	NIST Webbook
hvap	107.25	kJ/mol	Cheméo Relay (1.0)
ie	9.25	eV	Cheméo Relay (1.0)
log10ws	-4.76		Cheméo Relay (1.0)
logp	3.898		Crippen Method
mcvol	191.800	ml/mol	McGowan Method
pc	2287.14	kPa	Joback Method
tb	597.86	K	Cheméo Relay (1.0)
tc	814.66	K	Cheméo Relay (1.0)
tf	376.00 ± 1.00	K	NIST Webbook
vc	0.708	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	527.16	J/mol×K	697.43	Joback Method
cpg	540.70	J/mol×K	729.48	Joback Method

cpg	553.48	J/mol×K	761.53	Joback Method
cpg	565.53	J/mol×K	793.58	Joback Method
cpg	576.88	J/mol×K	825.63	Joback Method
cpg	587.57	J/mol×K	857.68	Joback Method
cpg	597.61	J/mol×K	889.73	Joback Method
dvisc	0.0022271	Pa×s	397.23	Joback Method
dvisc	0.0008134	Pa×s	447.26	Joback Method
dvisc	0.0003638	Pa×s	497.30	Joback Method
dvisc	0.0001885	Pa×s	547.33	Joback Method
dvisc	0.0001091	Pa×s	597.36	Joback Method
dvisc	0.0000687	Pa×s	647.40	Joback Method
dvisc	0.0000462	Pa×s	697.43	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.20363e+01
Coeff. B	-3.91173e+03
Coeff. C	-9.40500e+01
Temperature range (K), min.	427.00
Temperature range (K), max.	675.73

Sources

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0, beta):

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=C38350877&Units=SI

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Thermodynamic study of the sublimation of eight 4-n-alkylbenzoic acids: https://www.doi.org/10.1016/j.jct.2004.02.001

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
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