2-PROPYLCYCLOHEXANOL

Other names: trans-2-Propylcyclohexanol
Inchi: InChI=1S/C9H18O/c1-2-5-8-6-3-4-7-9(8)10/h8-10H,2-7H2,1H3
InchiKey: VZBNUCDUQJCIDP-UHFFFAOYSA-N
Formula: C9H18O
SMILES: CCCC1CCCCC1O
Mol. weight [g/mol]: 142.24
CAS: 5846-43-5

Physical Properties

Property code	Value	Unit	Source
af	0.5212		Cheméo Relay (1.0)
gf	-95.18	kJ/mol	Joback Method
hf	-329.27	kJ/mol	Cheméo Relay (1.0)
hfus	16.06	kJ/mol	Joback Method
hvap	70.42	kJ/mol	Cheméo Relay (1.0)
ie	9.56	eV	Cheméo Relay (1.0)
log10ws	-2.42		Cheméo Relay (1.0)
logp	2.338		Crippen Method
mcvol	132.680	ml/mol	McGowan Method
pc	3025.61	kPa	Joback Method
rinpol	1138.00		NIST Webbook
rinpol	1138.00		NIST Webbook
tb	478.23	K	Cheméo Relay (1.0)
tc	683.70	K	Cheméo Relay (1.0)
tf	256.75	K	Cheméo Relay (1.0)
vc	0.465	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	321.51	J/mol×K	512.38	Joback Method
cpg	406.60	J/mol×K	700.47	Joback Method
cpg	394.18	J/mol×K	669.12	Joback Method
cpg	381.07	J/mol×K	637.77	Joback Method

cpg	367.27	J/mol×K	606.42	Joback Method
cpg	352.75	J/mol×K	575.08	Joback Method
cpg	337.50	J/mol×K	543.73	Joback Method
dvisc	0.0009760	Pa×s	383.76	Joback Method
dvisc	0.0001611	Pa×s	512.38	Joback Method
dvisc	0.0002632	Pa×s	469.51	Joback Method
dvisc	0.0004745	Pa×s	426.64	Joback Method
dvisc	0.0363477	Pa×s	255.15	Joback Method
dvisc	0.0024066	Pa×s	340.89	Joback Method
dvisc	0.0076936	Pa×s	298.02	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.38284e+01
Coeff. B	-3.82131e+03
Coeff. C	-6.80910e+01
Temperature range (K), min.	350.30
Temperature range (K), max.	516.76

Sources

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

Cheméo Relay (1.0):

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=C90676258&Units=SI

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

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
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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume