2,4,6-Trichlorobenzyl alcohol, 1-methylpropyl ether

Inchi: InChI=1S/C11H13Cl3O/c1-3-7(2)15-6-9-10(13)4-8(12)5-11(9)14/h4-5,7H,3,6H2,1-2H3
InchiKey: DQTJCTRPYGVCLF-UHFFFAOYSA-N
Formula: C11H13Cl3O
SMILES: CCC(C)OCc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 267.58

Physical Properties

Property code	Value	Unit	Source
gf	-17.97	kJ/mol	Joback Method
hf	-252.97	kJ/mol	Joback Method
hfus	27.38	kJ/mol	Joback Method
hvap	59.52	kJ/mol	Joback Method
log10ws	-5.28		Crippen Method
logp	4.962		Crippen Method
mcvol	184.680	ml/mol	McGowan Method
pc	2250.40	kPa	Joback Method
rinpol	1662.00		NIST Webbook
tb	626.97	K	Joback Method
tc	847.93	K	Joback Method
tf	374.70	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.09	J/mol×K	626.97	Joback Method
cpg	463.32	J/mol×K	811.10	Joback Method
cpg	453.51	J/mol×K	774.28	Joback Method
cpg	443.00	J/mol×K	737.45	Joback Method
cpg	431.76	J/mol×K	700.62	Joback Method
cpg	419.80	J/mol×K	663.80	Joback Method
cpg	472.44	J/mol×K	847.93	Joback Method
dvisc	0.0001484	Pa×s	626.97	Joback Method
dvisc	0.0001845	Pa×s	584.92	Joback Method

dvisc	0.0002373	Pa×s	542.88	Joback Method
dvisc	0.0003183	Pa×s	500.84	Joback Method
dvisc	0.0004506	Pa×s	458.79	Joback Method
dvisc	0.0006843	Pa×s	416.75	Joback Method
dvisc	0.0011413	Pa×s	374.70	Joback Method

Sources

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

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

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U375275&Units=SI

Legend

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
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
pc: Critical Pressure
rinpol: Non-polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume

Latest version available from:
https://www.chemeo.com/cid/91-091-0/2-4-6-Trichlorobenzyl-alcohol-1-methylpropyl-ether.pdf
Generated by Cheméo on 2024-04-30 00:13:26.119992602 +0000 UTC m=+16725255.040569913.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.