Pentaerythrol monochlorohydrin

Inchi: InChI=1S/C5H11ClO3/c6-1-5(2-7,3-8)4-9/h7-9H,1-4H2
InchiKey: SJPSAGFZHAWRNW-UHFFFAOYSA-N
Formula: C5H11ClO3
SMILES: OCC(CO)(CO)CCl
Mol. weight [g/mol]: 154.59

Physical Properties

Property code	Value	Unit	Source
gf	-428.33	kJ/mol	Joback Method
hf	-627.71	kJ/mol	Joback Method
hfus	17.75	kJ/mol	Joback Method
hvap	79.85	kJ/mol	Joback Method
log10ws	0.38		Crippen Method
logp	-0.811		Crippen Method
mcvol	111.160	ml/mol	McGowan Method
pc	4822.53	kPa	Joback Method
rinpol	1500.00		NIST Webbook
rinpol	1500.00		NIST Webbook
tb	624.54	K	Joback Method
tc	791.78	K	Joback Method
tf	360.91	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	279.47	J/mol×K	624.54	Joback Method
cpg	308.09	J/mol×K	763.90	Joback Method
cpg	302.97	J/mol×K	736.03	Joback Method
cpg	297.57	J/mol×K	708.16	Joback Method
cpg	291.86	J/mol×K	680.29	Joback Method
cpg	285.84	J/mol×K	652.41	Joback Method
cpg	312.95	J/mol×K	791.78	Joback Method
dvisc	0.0000105	Pa×s	624.54	Joback Method

dvisc	0.0000227	Pa×s	580.60	Joback Method
dvisc	0.0000555	Pa×s	536.66	Joback Method
dvisc	0.0001594	Pa×s	492.73	Joback Method
dvisc	0.0005633	Pa×s	448.79	Joback Method
dvisc	0.0026171	Pa×s	404.85	Joback Method
dvisc	0.0176749	Pa×s	360.91	Joback Method

Sources

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=R490023&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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