1,3-Propanediol, bis(chlorodifluoroacetate)

Inchi: InChI=1S/C7H6Cl2F4O4/c8-6(10,11)4(14)16-2-1-3-17-5(15)7(9,12)13/h1-3H2
InchiKey: CJRWBYULDAAFPD-UHFFFAOYSA-N
Formula: C7H6Cl2F4O4
SMILES: O=C(OCCCOC(=O)C(F)(F)Cl)C(F)(F)Cl
Mol. weight [g/mol]: 301.02

Physical Properties

Property code	Value	Unit	Source
gf	-1257.20	kJ/mol	Joback Method
hf	-1510.83	kJ/mol	Joback Method
hfus	25.35	kJ/mol	Joback Method
hvap	52.40	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.126		Crippen Method
mcvol	155.930	ml/mol	McGowan Method
pc	2465.36	kPa	Joback Method
rinpol	1160.00		NIST Webbook
tb	577.62	K	Joback Method
tc	759.58	K	Joback Method
tf	380.01	K	Joback Method
vc	0.624	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	366.93	J/mol×K	577.62	Joback Method
cpg	375.58	J/mol×K	607.95	Joback Method
cpg	383.65	J/mol×K	638.27	Joback Method
cpg	391.17	J/mol×K	668.60	Joback Method
cpg	398.16	J/mol×K	698.93	Joback Method
cpg	404.63	J/mol×K	729.25	Joback Method
cpg	410.62	J/mol×K	759.58	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=U375555&Units=SI

Legend

cpg:	Ideal gas heat capacity
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