Octacosyl pentafluoropropionate

Other names: Octacosyl 2,2,3,3,3-pentafluoropropanoate
1-Octacosanol, pentafluoropropionate
Inchi: InChI=1S/C31H57F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey: MGPJOTUWJUFUCV-UHFFFAOYSA-N
Formula: C31H57F5O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 556.78

Physical Properties

Property code	Value	Unit	Source
gf	-992.15	kJ/mol	Joback Method
hf	-1926.02	kJ/mol	Joback Method
hfus	79.40	kJ/mol	Joback Method
hvap	87.08	kJ/mol	Joback Method
log10ws	-12.64		Crippen Method
logp	11.890		Crippen Method
mcvol	463.940	ml/mol	McGowan Method
pc	532.13	kPa	Joback Method
rinpol	2965.30		NIST Webbook
tb	974.86	K	Joback Method
tc	1234.96	K	Joback Method
tf	519.08	K	Joback Method
vc	1.863	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1647.80	J/mol×K	974.86	Joback Method
cpg	1676.08	J/mol×K	1018.21	Joback Method
cpg	1702.34	J/mol×K	1061.56	Joback Method
cpg	1726.82	J/mol×K	1104.91	Joback Method
cpg	1749.74	J/mol×K	1148.26	Joback Method
cpg	1771.32	J/mol×K	1191.61	Joback Method
cpg	1791.80	J/mol×K	1234.96	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=U351889&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