Dotriacontyl pentafluoropropionate

Other names: Dotriacontyl 2,2,3,3,3-pentafluoropropanoate
1-Dotriacontanol, pentafluoropropionate
Inchi: InChI=1S/C35H65F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey: QJTLRFYOMMIMKF-UHFFFAOYSA-N
Formula: C35H65F5O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 612.88

Physical Properties

Property code	Value	Unit	Source
gf	-958.47	kJ/mol	Joback Method
hf	-2008.58	kJ/mol	Joback Method
hfus	89.77	kJ/mol	Joback Method
hvap	95.98	kJ/mol	Joback Method
log10ws	-14.31		Crippen Method
logp	13.450		Crippen Method
mcvol	520.300	ml/mol	McGowan Method
pc	449.06	kPa	Joback Method
rinpol	3351.40		NIST Webbook
tb	1066.38	K	Joback Method
tc	1405.67	K	Joback Method
tf	564.16	K	Joback Method
vc	2.087	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1917.01	J/mol×K	1066.38	Joback Method
cpg	1952.61	J/mol×K	1122.93	Joback Method
cpg	1985.35	J/mol×K	1179.48	Joback Method
cpg	2015.79	J/mol×K	1236.02	Joback Method
cpg	2044.48	J/mol×K	1292.57	Joback Method
cpg	2071.99	J/mol×K	1349.12	Joback Method
cpg	2098.86	J/mol×K	1405.67	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351814&Units=SI
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

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