Hexatriacontyl pentafluoropropionate

Other names:	Hexatriacontyl 2,2,3,3,3-pentafluoropropanoate
	1-Hexatriacontanol, pentafluoropropionate
Inchi:	InChI=1S/C39H73F5O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	LOCRWHYJIWHMIX-UHFFFAOYSA-N
Formula:	C39H73F5O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	668.99

Physical Properties

Property code	Value	Unit	Source
gf	-924.79	kJ/mol	Joback Method
hf	-2091.14	kJ/mol	Joback Method
hfus	100.12	kJ/mol	Joback Method
hvap	104.89	kJ/mol	Joback Method
log10ws	-15.99		Crippen Method
logp	15.011		Crippen Method
mcvol	576.660	ml/mol	McGowan Method
pc	384.02	kPa	Joback Method
rinpol	3742.40		NIST Webbook
tb	1157.90	K	Joback Method
tc	1616.18	K	Joback Method
tf	609.24	K	Joback Method
vc	2.312	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2191.68	J/mol×K	1157.90	Joback Method
cpg	2238.27	J/mol×K	1234.28	Joback Method
cpg	2281.17	J/mol×K	1310.66	Joback Method
cpg	2321.86	J/mol×K	1387.04	Joback Method
cpg	2361.86	J/mol×K	1463.42	Joback Method
cpg	2402.66	J/mol×K	1539.80	Joback Method
cpg	2445.76	J/mol×K	1616.18	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351890&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

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