Hexatriacontyl trifluoroacetate

Other names:	Hexatriacontyl 2,2,2-trifluoroacetate
	1-Hexatriacontanol, trifluoroacetate
Inchi:	InChI=1S/C38H73F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	QUYZHXAAZPERTE-UHFFFAOYSA-N
Formula:	C38H73F3O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	618.98

Physical Properties

Property code	Value	Unit	Source
gf	-546.43	kJ/mol	Joback Method
hf	-1669.53	kJ/mol	Joback Method
hfus	98.79	kJ/mol	Joback Method
hvap	105.59	kJ/mol	Joback Method
log10ws	-15.25		Crippen Method
logp	14.375		Crippen Method
mcvol	559.030	ml/mol	McGowan Method
pc	410.44	kPa	Joback Method
rinpol	3776.90		NIST Webbook
tb	1139.71	K	Joback Method
tc	1552.91	K	Joback Method
tf	594.37	K	Joback Method
vc	2.231	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2110.31	J/mol×K	1139.71	Joback Method
cpg	2151.51	J/mol×K	1208.58	Joback Method
cpg	2188.48	J/mol×K	1277.44	Joback Method
cpg	2222.13	J/mol×K	1346.31	Joback Method
cpg	2253.39	J/mol×K	1415.18	Joback Method
cpg	2283.16	J/mol×K	1484.04	Joback Method
cpg	2312.35	J/mol×K	1552.91	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351886&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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