Tetratriacontyl trifluoroacetate

Other names:	Tetratriacontyl 2,2,2-trifluoroacetate
	1-Tetratriacontanol, trifluoroacetate
Inchi:	InChI=1S/C36H69F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey:	QCBQCHOKZRMGJL-UHFFFAOYSA-N
Formula:	C36H69F3O2
SMILES:	CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]:	590.93

Physical Properties

Property code	Value	Unit	Source
gf	-563.27	kJ/mol	Joback Method
hf	-1628.25	kJ/mol	Joback Method
hfus	93.61	kJ/mol	Joback Method
hvap	101.14	kJ/mol	Joback Method
log10ws	-14.42		Crippen Method
logp	13.595		Crippen Method
mcvol	530.850	ml/mol	McGowan Method
pc	444.34	kPa	Joback Method
rinpol	3570.50		NIST Webbook
rinpol	3570.50		NIST Webbook
tb	1093.95	K	Joback Method
tc	1450.37	K	Joback Method
tf	571.83	K	Joback Method
vc	2.119	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1973.17	J/mol×K	1093.95	Joback Method
cpg	2009.75	J/mol×K	1153.35	Joback Method
cpg	2042.83	J/mol×K	1212.76	Joback Method
cpg	2072.96	J/mol×K	1272.16	Joback Method
cpg	2100.70	J/mol×K	1331.56	Joback Method
cpg	2126.61	J/mol×K	1390.97	Joback Method

cpg	2151.23	J/mol×K	1450.37	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=U351753&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

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