Dotriacontyl trifluoroacetate

Other names: Dotriacontyl 2,2,2-trifluoroacetate
1-Dotriacontanol, trifluoroacetate
Inchi: InChI=1S/C34H65F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey: ZKTKQWPZEBJTKD-UHFFFAOYSA-N
Formula: C34H65F3O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 562.87

Physical Properties

Property code	Value	Unit	Source
gf	-580.11	kJ/mol	Joback Method
hf	-1586.97	kJ/mol	Joback Method
hfus	88.43	kJ/mol	Joback Method
hvap	96.69	kJ/mol	Joback Method
log10ws	-13.58		Crippen Method
logp	12.815		Crippen Method
mcvol	502.670	ml/mol	McGowan Method
pc	482.61	kPa	Joback Method
rinpol	3371.30		NIST Webbook
tb	1048.19	K	Joback Method
tc	1358.23	K	Joback Method
tf	549.29	K	Joback Method
vc	2.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1837.04	J/mol×K	1048.19	Joback Method
cpg	1869.77	J/mol×K	1099.86	Joback Method
cpg	1899.64	J/mol×K	1151.54	Joback Method
cpg	1926.98	J/mol×K	1203.21	Joback Method
cpg	1952.15	J/mol×K	1254.88	Joback Method
cpg	1975.50	J/mol×K	1306.55	Joback Method
cpg	1997.35	J/mol×K	1358.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351754&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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