Triacontyl trifluoroacetate

Other names: Triacontyl 2,2,2-trifluoroacetate
1-Triacontanol, trifluoroacetate
Inchi: InChI=1S/C32H61F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey: JDQMFLCNFDDCAA-UHFFFAOYSA-N
Formula: C32H61F3O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 534.82

Physical Properties

Property code	Value	Unit	Source
gf	-596.95	kJ/mol	Joback Method
hf	-1545.69	kJ/mol	Joback Method
hfus	83.25	kJ/mol	Joback Method
hvap	92.23	kJ/mol	Joback Method
log10ws	-12.74		Crippen Method
logp	12.035		Crippen Method
mcvol	474.490	ml/mol	McGowan Method
pc	526.05	kPa	Joback Method
rinpol	3173.70		NIST Webbook
rinpol	3173.70		NIST Webbook
tb	1002.43	K	Joback Method
tc	1274.78	K	Joback Method
tf	526.75	K	Joback Method
vc	1.895	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1702.09	J/mol×K	1002.43	Joback Method
cpg	1731.60	J/mol×K	1047.82	Joback Method
cpg	1758.77	J/mol×K	1093.21	Joback Method
cpg	1783.82	J/mol×K	1138.60	Joback Method
cpg	1806.97	J/mol×K	1184.00	Joback Method
cpg	1828.44	J/mol×K	1229.39	Joback Method

cpg	1848.45	J/mol×K	1274.78	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351757&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