Octatriacontyl trifluoroacetate

Other names: Octatriacontyl 2,2,2-trifluoroacetate
1-Octatriacontanol, trifluoroacetate
Inchi: InChI=1S/C40H77F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey: ADEIGZUMFHUKED-UHFFFAOYSA-N
Formula: C40H77F3O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 647.03

Physical Properties

Property code	Value	Unit	Source
gf	-529.59	kJ/mol	Joback Method
hf	-1710.81	kJ/mol	Joback Method
hfus	103.97	kJ/mol	Joback Method
hvap	110.04	kJ/mol	Joback Method
log10ws	-16.09		Crippen Method
logp	15.155		Crippen Method
mcvol	587.210	ml/mol	McGowan Method
pc	380.28	kPa	Joback Method
rinpol	3975.40		NIST Webbook
rinpol	3975.40		NIST Webbook
tb	1185.47	K	Joback Method
tc	1667.97	K	Joback Method
tf	616.91	K	Joback Method
vc	2.342	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	2248.37	J/mol×K	1185.47	Joback Method
cpg	2295.16	J/mol×K	1265.89	Joback Method
cpg	2336.98	J/mol×K	1346.30	Joback Method
cpg	2375.37	J/mol×K	1426.72	Joback Method
cpg	2411.84	J/mol×K	1507.14	Joback Method
cpg	2447.94	J/mol×K	1587.55	Joback Method

cpg	2485.17	J/mol×K	1667.97	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=U351887&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