Octacosyl trifluoroacetate

Other names: Octacosyl 2,2,2-trifluoroacetate
1-Octacosanol, trifluoroacetate
Inchi: InChI=1S/C30H57F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-22-23
InchiKey: DBJWKKYWNRSCGQ-UHFFFAOYSA-N
Formula: C30H57F3O2
SMILES: CCCCCCCCCCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 506.77

Physical Properties

Property code	Value	Unit	Source
gf	-613.79	kJ/mol	Joback Method
hf	-1504.41	kJ/mol	Joback Method
hfus	78.07	kJ/mol	Joback Method
hvap	87.78	kJ/mol	Joback Method
log10ws	-11.91		Crippen Method
logp	11.254		Crippen Method
mcvol	446.310	ml/mol	McGowan Method
pc	575.63	kPa	Joback Method
rinpol	2974.70		NIST Webbook
rinpol	2974.70		NIST Webbook
tb	956.67	K	Joback Method
tc	1198.66	K	Joback Method
tf	504.21	K	Joback Method
vc	1.782	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1568.53	J/mol×K	956.67	Joback Method
cpg	1595.34	J/mol×K	997.00	Joback Method
cpg	1620.23	J/mol×K	1037.33	Joback Method
cpg	1643.34	J/mol×K	1077.66	Joback Method
cpg	1664.82	J/mol×K	1117.99	Joback Method
cpg	1684.82	J/mol×K	1158.32	Joback Method

cpg	1703.48	J/mol×K	1198.66	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351749&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