Eicosyl trifluoroacetate

Other names: Eicosyl 2,2,2-trifluoroacetate
1-Eicosanol, trifluoroacetate
Inchi: InChI=1S/C22H41F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-27-21(26
InchiKey: JELHWUPDJFSSDO-UHFFFAOYSA-N
Formula: C22H41F3O2
SMILES: CCCCCCCCCCCCCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 394.55

Physical Properties

Property code	Value	Unit	Source
gf	-681.15	kJ/mol	Joback Method
hf	-1339.29	kJ/mol	Joback Method
hfus	57.35	kJ/mol	Joback Method
hvap	69.98	kJ/mol	Joback Method
log10ws	-8.56		Crippen Method
logp	8.134		Crippen Method
mcvol	333.590	ml/mol	McGowan Method
pc	865.05	kPa	Joback Method
rinpol	2201.00		NIST Webbook
rinpol	2201.00		NIST Webbook
tb	773.63	K	Joback Method
tc	947.38	K	Joback Method
tf	414.05	K	Joback Method
vc	1.335	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1054.40	J/mol×K	773.63	Joback Method
cpg	1074.22	J/mol×K	802.59	Joback Method
cpg	1093.03	J/mol×K	831.55	Joback Method
cpg	1110.87	J/mol×K	860.51	Joback Method
cpg	1127.78	J/mol×K	889.47	Joback Method
cpg	1143.81	J/mol×K	918.43	Joback Method

cpg	1158.99	J/mol×K	947.38	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U351752&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