Oleyl alcohol, trifluoroacetate

Inchi: InChI=1S/C20H35F3O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-25-19(24)20(21
InchiKey: FLDNEOWDJOPXSX-KTKRTIGZSA-N
Formula: C20H35F3O2
SMILES: CCCCCCCCC=CCCCCCCCCOC(=O)C(F)(F)F
Mol. weight [g/mol]: 364.49

Physical Properties

Property code	Value	Unit	Source
gf	-617.77	kJ/mol	Joback Method
hf	-1180.79	kJ/mol	Joback Method
hfus	52.37	kJ/mol	Joback Method
hvap	65.48	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	7.129		Crippen Method
mcvol	301.110	ml/mol	McGowan Method
pc	1003.98	kPa	Joback Method
rinpol	1990.40		NIST Webbook
tb	732.03	K	Joback Method
tc	900.77	K	Joback Method
tf	386.43	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.93	J/mol×K	732.03	Joback Method
cpg	928.04	J/mol×K	760.15	Joback Method
cpg	945.28	J/mol×K	788.28	Joback Method
cpg	961.66	J/mol×K	816.40	Joback Method
cpg	977.25	J/mol×K	844.52	Joback Method
cpg	992.08	J/mol×K	872.65	Joback Method
cpg	1006.18	J/mol×K	900.77	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352684&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