Oleyl alcohol, heptafluorobutyrate

Inchi: InChI=1S/C22H35F7O2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-31-19(30)20(23
InchiKey: TYNFPJQYUUJEMG-KTKRTIGZSA-N
Formula: C22H35F7O2
SMILES: CCCCCCCCC=CCCCCCCCCCOC(=O)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 464.50

Physical Properties

Property code	Value	Unit	Source
gf	-1374.49	kJ/mol	Joback Method
hf	-2024.01	kJ/mol	Joback Method
hfus	55.04	kJ/mol	Joback Method
hvap	64.07	kJ/mol	Joback Method
log10ws	-9.04		Crippen Method
logp	8.400		Crippen Method
mcvol	336.370	ml/mol	McGowan Method
pc	821.01	kPa	Joback Method
rinpol	2019.20		NIST Webbook
tb	768.41	K	Joback Method
tc	940.80	K	Joback Method
tf	416.17	K	Joback Method
vc	1.365	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1062.74	J/mol×K	768.41	Joback Method
cpg	1080.86	J/mol×K	797.14	Joback Method
cpg	1098.01	J/mol×K	825.87	Joback Method
cpg	1114.25	J/mol×K	854.60	Joback Method
cpg	1129.67	J/mol×K	883.34	Joback Method
cpg	1144.32	J/mol×K	912.07	Joback Method
cpg	1158.28	J/mol×K	940.80	Joback Method

Sources

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=U352681&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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