Cycloheptanol, heptafluorobutyrate

Inchi: InChI=1S/C11H13F7O2/c12-9(13,10(14,15)11(16,17)18)8(19)20-7-5-3-1-2-4-6-7/h7H,1-6
InchiKey: JHDGOBLRISUXNP-UHFFFAOYSA-N
Formula: C11H13F7O2
SMILES: O=C(OC1CCCCCC1)C(F)(F)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 310.21

Physical Properties

Property code	Value	Unit	Source
gf	-1534.98	kJ/mol	Joback Method
hf	-1866.03	kJ/mol	Joback Method
hfus	16.09	kJ/mol	Joback Method
hvap	40.23	kJ/mol	Joback Method
log10ws	-4.59		Crippen Method
logp	4.085		Crippen Method
mcvol	174.820	ml/mol	McGowan Method
pc	1964.82	kPa	Joback Method
rinpol	1082.00		NIST Webbook
rinpol	1082.00		NIST Webbook
tb	536.39	K	Joback Method
tc	714.81	K	Joback Method
tf	301.14	K	Joback Method
vc	0.694	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	470.52	J/mol×K	536.39	Joback Method
cpg	487.51	J/mol×K	566.13	Joback Method
cpg	503.42	J/mol×K	595.86	Joback Method
cpg	518.28	J/mol×K	625.60	Joback Method
cpg	532.14	J/mol×K	655.34	Joback Method
cpg	545.05	J/mol×K	685.07	Joback Method
cpg	557.05	J/mol×K	714.81	Joback Method

Sources

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=U376256&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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