Cycloheptanol, pentafluoropropionate

Inchi: InChI=1S/C10H13F5O2/c11-9(12,10(13,14)15)8(16)17-7-5-3-1-2-4-6-7/h7H,1-6H2
InchiKey: FAZVYYMZEIGFFS-UHFFFAOYSA-N
Formula: C10H13F5O2
SMILES: O=C(OC1CCCCCC1)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 260.20

Physical Properties

Property code	Value	Unit	Source
gf	-1156.62	kJ/mol	Joback Method
hf	-1444.42	kJ/mol	Joback Method
hfus	14.75	kJ/mol	Joback Method
hvap	40.93	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.450		Crippen Method
mcvol	157.190	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
rinpol	1038.00		NIST Webbook
tb	518.20	K	Joback Method
tc	705.35	K	Joback Method
tf	286.27	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	402.45	J/mol×K	518.20	Joback Method
cpg	419.44	J/mol×K	549.39	Joback Method
cpg	435.40	J/mol×K	580.58	Joback Method
cpg	450.36	J/mol×K	611.78	Joback Method
cpg	464.37	J/mol×K	642.97	Joback Method
cpg	477.46	J/mol×K	674.16	Joback Method
cpg	489.66	J/mol×K	705.35	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=U376257&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