Pentafluoropropionic acid, heptyl ester

Other names: Heptyl pentafluoropropionate
Inchi: InChI=1S/C10H15F5O2/c1-2-3-4-5-6-7-17-8(16)9(11,12)10(13,14)15/h2-7H2,1H3
InchiKey: XVYGQEAPOGQAKL-UHFFFAOYSA-N
Formula: C10H15F5O2
SMILES: CCCCCCCOC(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]: 262.22
CAS: 959033-16-0

Physical Properties

Property code	Value	Unit	Source
gf	-1168.97	kJ/mol	Joback Method
hf	-1492.58	kJ/mol	Joback Method
hfus	25.02	kJ/mol	Joback Method
hvap	40.33	kJ/mol	Joback Method
log10ws	-3.85		Crippen Method
logp	3.698		Crippen Method
mcvol	168.050	ml/mol	McGowan Method
pc	1859.51	kPa	Joback Method
rinpol	989.00		NIST Webbook
rinpol	995.60		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	962.00		NIST Webbook
ripol	1025.00		NIST Webbook
ripol	1025.00		NIST Webbook
ripol	1016.00		NIST Webbook
tb	494.38	K	Joback Method
tc	647.68	K	Joback Method
tf	282.41	K	Joback Method
vc	0.688	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.79	J/mol×K	494.38	Joback Method

cpg	427.87	J/mol×K	519.93	Joback Method
cpg	440.32	J/mol×K	545.48	Joback Method
cpg	452.17	J/mol×K	571.03	Joback Method
cpg	463.44	J/mol×K	596.58	Joback Method
cpg	474.15	J/mol×K	622.13	Joback Method
cpg	484.31	J/mol×K	647.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C959033160&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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume