Hexyl 2,3,4,5,6-pentafluorobenzoate

Other names: hexyl pentafluorobenzoate
Inchi: InChI=1S/C13H13F5O2/c1-2-3-4-5-6-20-13(19)7-8(14)10(16)12(18)11(17)9(7)15/h2-6H2
InchiKey: WVNPCCPQMDSFOU-UHFFFAOYSA-N
Formula: C13H13F5O2
SMILES: CCCCCCOC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 296.23

Physical Properties

Property code	Value	Unit	Source
gf	-1085.13	kJ/mol	Joback Method
hf	-1357.82	kJ/mol	Joback Method
hfus	39.71	kJ/mol	Joback Method
hvap	55.19	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	4.119		Crippen Method
mcvol	186.560	ml/mol	McGowan Method
pc	1752.14	kPa	Joback Method
rinpol	1426.00		NIST Webbook
rinpol	1433.00		NIST Webbook
rinpol	1442.00		NIST Webbook
rinpol	1418.00		NIST Webbook
rinpol	1410.00		NIST Webbook
rinpol	1419.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1417.00		NIST Webbook
rinpol	1419.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1704.00		NIST Webbook
ripol	1723.00		NIST Webbook
ripol	1695.00		NIST Webbook
ripol	1720.00		NIST Webbook
ripol	1673.00		NIST Webbook
ripol	1688.00		NIST Webbook
ripol	1705.00		NIST Webbook
tb	621.06	K	Joback Method
tc	790.96	K	Joback Method
tf	400.40	K	Joback Method

vc	0.769	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	481.72	J/mol×K	621.06	Joback Method
cpg	493.60	J/mol×K	649.38	Joback Method
cpg	504.97	J/mol×K	677.69	Joback Method
cpg	515.83	J/mol×K	706.01	Joback Method
cpg	526.19	J/mol×K	734.33	Joback Method
cpg	536.05	J/mol×K	762.65	Joback Method
cpg	545.42	J/mol×K	790.96	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U373590&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