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

Inchi: InChI=1S/C12H11F5O2/c1-12(2,3)4-19-11(18)5-6(13)8(15)10(17)9(16)7(5)14/h4H2,1-3H
InchiKey: AAOFTXNPZBGMJK-UHFFFAOYSA-N
Formula: C12H11F5O2
SMILES: CC(C)(C)COC(=O)c1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 282.21

Physical Properties

Property code	Value	Unit	Source
gf	-1090.71	kJ/mol	Joback Method
hf	-1345.93	kJ/mol	Joback Method
hfus	29.71	kJ/mol	Joback Method
hvap	51.67	kJ/mol	Joback Method
log10ws	-4.80		Crippen Method
logp	3.585		Crippen Method
mcvol	172.470	ml/mol	McGowan Method
pc	1933.83	kPa	Joback Method
rinpol	1247.00		NIST Webbook
tb	594.95	K	Joback Method
tc	773.60	K	Joback Method
tf	391.55	K	Joback Method
vc	0.703	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	436.19	J/mol×K	594.95	Joback Method
cpg	447.80	J/mol×K	624.73	Joback Method
cpg	458.84	J/mol×K	654.50	Joback Method
cpg	469.33	J/mol×K	684.28	Joback Method
cpg	479.27	J/mol×K	714.05	Joback Method
cpg	488.67	J/mol×K	743.83	Joback Method
cpg	497.55	J/mol×K	773.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373601&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume