2,5-Difluorobenzoic acid, neopentyl ester

Inchi: InChI=1S/C12H14F2O2/c1-12(2,3)7-16-11(15)9-6-8(13)4-5-10(9)14/h4-6H,7H2,1-3H3
InchiKey: FMSSMYKYTBRTDG-UHFFFAOYSA-N
Formula: C12H14F2O2
SMILES: CC(C)(C)COC(=O)c1cc(F)ccc1F
Mol. weight [g/mol]: 228.24

Physical Properties

Property code	Value	Unit	Source
gf	-477.39	kJ/mol	Joback Method
hf	-723.19	kJ/mol	Joback Method
hfus	21.63	kJ/mol	Joback Method
hvap	52.13	kJ/mol	Joback Method
log10ws	-3.81		Crippen Method
logp	3.168		Crippen Method
mcvol	167.160	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	1341.00		NIST Webbook
tb	582.20	K	Joback Method
tc	782.68	K	Joback Method
tf	352.22	K	Joback Method
vc	0.648	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	413.12	J/mol×K	582.20	Joback Method
cpg	427.17	J/mol×K	615.61	Joback Method
cpg	440.40	J/mol×K	649.03	Joback Method
cpg	452.84	J/mol×K	682.44	Joback Method
cpg	464.51	J/mol×K	715.85	Joback Method
cpg	475.45	J/mol×K	749.27	Joback Method
cpg	485.68	J/mol×K	782.68	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=U357572&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