2,6-Difluoro-3-methylbenzoic acid, neopentyl ester

Inchi: InChI=1S/C13H16F2O2/c1-8-5-6-9(14)10(11(8)15)12(16)17-7-13(2,3)4/h5-6H,7H2,1-4H3

InchiKey: MFRFHODKXZORNB-UHFFFAOYSA-N

Formula: C13H16F2O2

SMILES: Cc1ccc(F)c(C(=O)OCC(C)(C)C)c1F

Mol. weight [g/mol]: 242.26

Physical Properties

Property code	Value	Unit	Source
gf	-478.60	kJ/mol	Joback Method
hf	-755.30	kJ/mol	Joback Method
hfus	23.83	kJ/mol	Joback Method
hvap	55.02	kJ/mol	Joback Method
log10ws	-4.29		Crippen Method
logp	3.476		Crippen Method
mcvol	181.250	ml/mol	McGowan Method
pc	2056.76	kPa	Joback Method
rinpol	1482.00		NIST Webbook
tb	610.06	K	Joback Method
tc	808.72	K	Joback Method
tf	376.01	K	Joback Method
vc	0.705	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	461.70	J/mol×K	610.06	Joback Method
cpg	476.14	J/mol×K	643.17	Joback Method
cpg	489.77	J/mol×K	676.28	Joback Method
cpg	502.62	J/mol×K	709.39	Joback Method
cpg	514.70	J/mol×K	742.50	Joback Method
cpg	526.05	J/mol×K	775.61	Joback Method
cpg	536.69	J/mol×K	808.72	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=U357674&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

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