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

Inchi: InChI=1S/C15H7F7O2/c1-5-2-3-7(16)8(9(5)17)15(23)24-4-6-10(18)12(20)14(22)13(21)11

InchiKey: OAEQDGGSEUOFOB-UHFFFAOYSA-N

Formula: C15H7F7O2

SMILES: Cc1ccc(F)c(C(=O)OCc2c(F)c(F)c(F)c(F)c2F)c1F

Mol. weight [g/mol]: 352.20

Physical Properties

Property code	Value	Unit	Source
gf	-1374.39	kJ/mol	Joback Method
hf	-1589.20	kJ/mol	Joback Method
hfus	43.92	kJ/mol	Joback Method
hvap	62.27	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	4.326		Crippen Method
mcvol	194.520	ml/mol	McGowan Method
pc	1758.02	kPa	Joback Method
rinpol	1773.00		NIST Webbook
rinpol	1773.00		NIST Webbook
tb	706.98	K	Joback Method
tc	892.69	K	Joback Method
tf	488.10	K	Joback Method
vc	0.809	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	513.72	J/mol×K	706.98	Joback Method
cpg	524.23	J/mol×K	737.93	Joback Method
cpg	534.13	J/mol×K	768.88	Joback Method
cpg	543.42	J/mol×K	799.83	Joback Method
cpg	552.11	J/mol×K	830.78	Joback Method
cpg	560.19	J/mol×K	861.74	Joback Method
cpg	567.66	J/mol×K	892.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343754&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