2,6-Difluoro-3-methylbenzoic acid, 2,2,3,3,4,4,4-heptafluorobutyl ester

Inchi: InChI=1S/C12H7F9O2/c1-5-2-3-6(13)7(8(5)14)9(22)23-4-10(15,16)11(17,18)12(19,20)21

InchiKey: CXTFXSRUMLMKOH-UHFFFAOYSA-N

Formula: C12H7F9O2

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

Mol. weight [g/mol]: 354.17

Physical Properties

Property code	Value	Unit	Source
gf	-1845.01	kJ/mol	Joback Method
hf	-2124.93	kJ/mol	Joback Method
hfus	27.97	kJ/mol	Joback Method
hvap	44.48	kJ/mol	Joback Method
log10ws	-5.40		Crippen Method
logp	4.263		Crippen Method
mcvol	179.550	ml/mol	McGowan Method
pc	1756.54	kPa	Joback Method
rinpol	1230.00		NIST Webbook
rinpol	1230.00		NIST Webbook
tb	575.61	K	Joback Method
tc	741.42	K	Joback Method
tf	373.71	K	Joback Method
vc	0.752	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	476.82	J/mol×K	575.61	Joback Method
cpg	488.03	J/mol×K	603.24	Joback Method
cpg	498.51	J/mol×K	630.88	Joback Method
cpg	508.30	J/mol×K	658.51	Joback Method
cpg	517.44	J/mol×K	686.15	Joback Method
cpg	525.95	J/mol×K	713.78	Joback Method
cpg	533.87	J/mol×K	741.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343748&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