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

Inchi: InChI=1S/C14H17ClF2O2/c1-10-6-7-11(16)12(13(10)17)14(18)19-9-5-3-2-4-8-15/h6-7H,

InchiKey: LIBCWLJDORTDFR-UHFFFAOYSA-N

Formula: C14H17ClF2O2

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

Mol. weight [g/mol]: 290.73

Physical Properties

Property code	Value	Unit	Source
gf	-484.95	kJ/mol	Joback Method
hf	-782.93	kJ/mol	Joback Method
hfus	38.03	kJ/mol	Joback Method
hvap	62.93	kJ/mol	Joback Method
log10ws	-5.10		Crippen Method
logp	4.229		Crippen Method
mcvol	207.580	ml/mol	McGowan Method
pc	1800.03	kPa	Joback Method
rinpol	2002.00		NIST Webbook
rinpol	2002.00		NIST Webbook
tb	673.60	K	Joback Method
tc	864.47	K	Joback Method
tf	414.78	K	Joback Method
vc	0.821	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	537.37	J/mol×K	673.60	Joback Method
cpg	550.96	J/mol×K	705.41	Joback Method
cpg	563.83	J/mol×K	737.22	Joback Method
cpg	575.98	J/mol×K	769.03	Joback Method
cpg	587.42	J/mol×K	800.84	Joback Method
cpg	598.18	J/mol×K	832.66	Joback Method
cpg	608.26	J/mol×K	864.47	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U343755&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

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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