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

Inchi: InChI=1S/C20H30F2O2/c1-3-4-5-6-7-8-9-10-11-12-15-24-20(23)18-17(21)14-13-16(2)19

InchiKey: FEGRDNZQEZNMQG-UHFFFAOYSA-N

Formula: C20H30F2O2

SMILES: CCCCCCCCCCCCOC(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 340.45

Physical Properties

Property code	Value	Unit	Source
gf	-422.50	kJ/mol	Joback Method
hf	-891.03	kJ/mol	Joback Method
hfus	49.38	kJ/mol	Joback Method
hvap	71.90	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.351		Crippen Method
mcvol	279.880	ml/mol	McGowan Method
pc	1192.35	kPa	Joback Method
rinpol	2308.00		NIST Webbook
rinpol	2308.00		NIST Webbook
tb	773.45	K	Joback Method
tc	957.68	K	Joback Method
tf	452.48	K	Joback Method
vc	1.107	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	840.70	J/mol×K	773.45	Joback Method
cpg	857.72	J/mol×K	804.16	Joback Method
cpg	873.80	J/mol×K	834.86	Joback Method
cpg	888.96	J/mol×K	865.57	Joback Method
cpg	903.24	J/mol×K	896.27	Joback Method
cpg	916.65	J/mol×K	926.98	Joback Method
cpg	929.20	J/mol×K	957.68	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338849&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