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

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

InchiKey: CNSYMOGEJAVVTN-UHFFFAOYSA-N

Formula: C20H30F2O2

SMILES: CCCCCCCCCC(CC)OC(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 340.45

Physical Properties

Property code	Value	Unit	Source
gf	-424.94	kJ/mol	Joback Method
hf	-896.31	kJ/mol	Joback Method
hfus	45.85	kJ/mol	Joback Method
hvap	71.51	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	6.349		Crippen Method
mcvol	279.880	ml/mol	McGowan Method
pc	1198.96	kPa	Joback Method
rinpol	2200.00		NIST Webbook
rinpol	2200.00		NIST Webbook
tb	773.01	K	Joback Method
tc	958.86	K	Joback Method
tf	437.48	K	Joback Method
vc	1.101	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	841.20	J/mol×K	773.01	Joback Method
cpg	858.37	J/mol×K	803.98	Joback Method
cpg	874.59	J/mol×K	834.96	Joback Method
cpg	889.86	J/mol×K	865.93	Joback Method
cpg	904.22	J/mol×K	896.91	Joback Method
cpg	917.69	J/mol×K	927.88	Joback Method
cpg	930.28	J/mol×K	958.86	Joback Method

Sources

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=U338581&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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