2,4-Difluorobenzoic acid, 2-dodecyl ester

Inchi: InChI=1S/C19H28F2O2/c1-3-4-5-6-7-8-9-10-11-15(2)23-19(22)17-13-12-16(20)14-18(17
InchiKey: FQTYXXPOMJOHON-UHFFFAOYSA-N
Formula: C19H28F2O2
SMILES: CCCCCCCCCCC(C)OC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 326.42

Physical Properties

Property code	Value	Unit	Source
gf	-423.73	kJ/mol	Joback Method
hf	-864.20	kJ/mol	Joback Method
hfus	43.65	kJ/mol	Joback Method
hvap	68.62	kJ/mol	Joback Method
log10ws	-7.09		Crippen Method
logp	6.041		Crippen Method
mcvol	265.790	ml/mol	McGowan Method
pc	1296.73	kPa	Joback Method
rinpol	2078.00		NIST Webbook
rinpol	2078.00		NIST Webbook
tb	745.15	K	Joback Method
tc	929.57	K	Joback Method
tf	413.69	K	Joback Method
vc	1.046	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	783.42	J/mol×K	745.15	Joback Method
cpg	800.35	J/mol×K	775.89	Joback Method
cpg	816.35	J/mol×K	806.62	Joback Method
cpg	831.44	J/mol×K	837.36	Joback Method
cpg	845.65	J/mol×K	868.10	Joback Method
cpg	859.00	J/mol×K	898.84	Joback Method
cpg	871.51	J/mol×K	929.57	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338562&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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