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

Inchi: InChI=1S/C18H26F2O2/c1-3-4-5-6-7-8-9-10-13-22-18(21)16-15(19)12-11-14(2)17(16)20
InchiKey: IYADFPCKZSRUAM-UHFFFAOYSA-N
Formula: C18H26F2O2
SMILES: CCCCCCCCCCOC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 312.39

Physical Properties

Property code	Value	Unit	Source
gf	-439.34	kJ/mol	Joback Method
hf	-849.75	kJ/mol	Joback Method
hfus	44.20	kJ/mol	Joback Method
hvap	67.45	kJ/mol	Joback Method
log10ws	-6.62		Crippen Method
logp	5.571		Crippen Method
mcvol	251.700	ml/mol	McGowan Method
pc	1367.69	kPa	Joback Method
rinpol	2102.00		NIST Webbook
rinpol	2102.00		NIST Webbook
tb	727.69	K	Joback Method
tc	910.80	K	Joback Method
tf	429.94	K	Joback Method
vc	0.996	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	725.56	J/mol×K	727.69	Joback Method
cpg	741.83	J/mol×K	758.21	Joback Method
cpg	757.25	J/mol×K	788.73	Joback Method
cpg	771.83	J/mol×K	819.24	Joback Method
cpg	785.60	J/mol×K	849.76	Joback Method
cpg	798.56	J/mol×K	880.28	Joback Method
cpg	810.73	J/mol×K	910.80	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338847&Units=SI

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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