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

Inchi: InChI=1S/C16H22F2O2/c1-4-6-7-12(5-2)10-20-16(19)14-13(17)9-8-11(3)15(14)18/h8-9,1

InchiKey: XIBTWSBPKABFMD-UHFFFAOYSA-N

Formula: C16H22F2O2

SMILES: CCCCC(CC)COC(=O)c1c(F)ccc(C)c1F

Mol. weight [g/mol]: 284.34

Physical Properties

Property code	Value	Unit	Source
gf	-458.62	kJ/mol	Joback Method
hf	-813.75	kJ/mol	Joback Method
hfus	35.49	kJ/mol	Joback Method
hvap	62.61	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.646		Crippen Method
mcvol	223.520	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	1824.00		NIST Webbook
tb	681.49	K	Joback Method
tc	868.28	K	Joback Method
tf	392.40	K	Joback Method
vc	0.877	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	615.30	J/mol×K	681.49	Joback Method
cpg	630.99	J/mol×K	712.62	Joback Method
cpg	645.87	J/mol×K	743.75	Joback Method
cpg	659.96	J/mol×K	774.89	Joback Method
cpg	673.26	J/mol×K	806.02	Joback Method
cpg	685.79	J/mol×K	837.15	Joback Method
cpg	697.56	J/mol×K	868.28	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=U357679&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

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