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

Inchi: InChI=1S/C15H20F2O2/c1-3-4-5-6-7-10-19-15(18)13-12(16)9-8-11(2)14(13)17/h8-9H,3-
InchiKey: MEJDHUSQBCNUTP-UHFFFAOYSA-N
Formula: C15H20F2O2
SMILES: CCCCCCCOC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]: 270.31

Physical Properties

Property code	Value	Unit	Source
gf	-464.60	kJ/mol	Joback Method
hf	-787.83	kJ/mol	Joback Method
hfus	36.43	kJ/mol	Joback Method
hvap	60.77	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.400		Crippen Method
mcvol	209.430	ml/mol	McGowan Method
pc	1713.19	kPa	Joback Method
rinpol	1796.00		NIST Webbook
rinpol	1796.00		NIST Webbook
tb	659.05	K	Joback Method
tc	844.29	K	Joback Method
tf	396.13	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.31	J/mol×K	659.05	Joback Method
cpg	576.27	J/mol×K	689.92	Joback Method
cpg	590.48	J/mol×K	720.80	Joback Method
cpg	603.97	J/mol×K	751.67	Joback Method
cpg	616.73	J/mol×K	782.55	Joback Method
cpg	628.78	J/mol×K	813.42	Joback Method
cpg	640.14	J/mol×K	844.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338844&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

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