2,4-Difluorobenzoic acid, octyl ester

Inchi: InChI=1S/C15H20F2O2/c1-2-3-4-5-6-7-10-19-15(18)13-9-8-12(16)11-14(13)17/h8-9,11H
InchiKey: NZACAHJMBMPJNC-UHFFFAOYSA-N
Formula: C15H20F2O2
SMILES: CCCCCCCCOC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 270.31

Physical Properties

Property code	Value	Unit	Source
gf	-454.97	kJ/mol	Joback Method
hf	-776.36	kJ/mol	Joback Method
hfus	36.82	kJ/mol	Joback Method
hvap	60.11	kJ/mol	Joback Method
log10ws	-5.31		Crippen Method
logp	4.482		Crippen Method
mcvol	209.430	ml/mol	McGowan Method
pc	1734.67	kPa	Joback Method
rinpol	1864.00		NIST Webbook
rinpol	1864.00		NIST Webbook
tb	654.07	K	Joback Method
tc	838.45	K	Joback Method
tf	383.61	K	Joback Method
vc	0.828	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	561.72	J/mol×K	654.07	Joback Method
cpg	576.83	J/mol×K	684.80	Joback Method
cpg	591.17	J/mol×K	715.53	Joback Method
cpg	604.76	J/mol×K	746.26	Joback Method
cpg	617.61	J/mol×K	776.99	Joback Method
cpg	629.74	J/mol×K	807.72	Joback Method
cpg	641.16	J/mol×K	838.45	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338786&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