2,4-Difluorobenzoic acid, heptyl ester

Inchi: InChI=1S/C14H18F2O2/c1-2-3-4-5-6-9-18-14(17)12-8-7-11(15)10-13(12)16/h7-8,10H,2-6
InchiKey: PORSASSLXZILRU-UHFFFAOYSA-N
Formula: C14H18F2O2
SMILES: CCCCCCCOC(=O)c1ccc(F)cc1F
Mol. weight [g/mol]: 256.29

Physical Properties

Property code	Value	Unit	Source
gf	-463.39	kJ/mol	Joback Method
hf	-755.72	kJ/mol	Joback Method
hfus	34.23	kJ/mol	Joback Method
hvap	57.88	kJ/mol	Joback Method
log10ws	-4.89		Crippen Method
logp	4.092		Crippen Method
mcvol	195.340	ml/mol	McGowan Method
pc	1882.17	kPa	Joback Method
rinpol	1660.00		NIST Webbook
rinpol	1660.00		NIST Webbook
tb	631.19	K	Joback Method
tc	817.08	K	Joback Method
tf	372.34	K	Joback Method
vc	0.771	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	509.59	J/mol×K	631.19	Joback Method
cpg	524.18	J/mol×K	662.17	Joback Method
cpg	538.04	J/mol×K	693.15	Joback Method
cpg	551.17	J/mol×K	724.13	Joback Method
cpg	563.60	J/mol×K	755.12	Joback Method
cpg	575.34	J/mol×K	786.10	Joback Method
cpg	586.41	J/mol×K	817.08	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=U338785&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