3,4-Difluorobenzoic acid, decyl ester

Inchi: InChI=1S/C17H24F2O2/c1-2-3-4-5-6-7-8-9-12-21-17(20)14-10-11-15(18)16(19)13-14/h1
InchiKey: BQPUIPCCEZZZAU-UHFFFAOYSA-N
Formula: C17H24F2O2
SMILES: CCCCCCCCCCOC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]: 298.37

Physical Properties

Property code	Value	Unit	Source
gf	-438.13	kJ/mol	Joback Method
hf	-817.64	kJ/mol	Joback Method
hfus	42.00	kJ/mol	Joback Method
hvap	64.56	kJ/mol	Joback Method
log10ws	-6.14		Crippen Method
logp	5.262		Crippen Method
mcvol	237.610	ml/mol	McGowan Method
pc	1487.29	kPa	Joback Method
rinpol	1957.00		NIST Webbook
rinpol	1957.00		NIST Webbook
tb	699.83	K	Joback Method
tc	882.34	K	Joback Method
tf	406.15	K	Joback Method
vc	0.940	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	669.96	J/mol×K	699.83	Joback Method
cpg	685.95	J/mol×K	730.25	Joback Method
cpg	701.10	J/mol×K	760.67	Joback Method
cpg	715.44	J/mol×K	791.09	Joback Method
cpg	728.99	J/mol×K	821.50	Joback Method
cpg	741.75	J/mol×K	851.92	Joback Method
cpg	753.76	J/mol×K	882.34	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=U338866&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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