

2,5-Difluorobenzoic acid, decyl ester

Inchi:	InChI=1S/C17H24F2O2/c1-2-3-4-5-6-7-8-9-12-21-17(20)15-13-14(18)10-11-16(15)19/h1
InchiKey:	SVYUMMBPQMUTEK-UHFFFAOYSA-N
Formula:	C17H24F2O2
SMILES:	CCCCCCCCCOC(=O)c1cc(F)ccc1F
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	1985.00		NIST Webbook
rinpol	1985.00		NIST Webbook
tb	699.83	K	Joback Method
tc	882.34	K	Joback Method
tf	406.15	K	Joback Method
vc	0.940	m ³ /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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U338809&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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