

3,4-Difluorobenzoic acid, 4-hexadecyl ester

Inchi:	InChI=1S/C23H36F2O2/c1-3-5-6-7-8-9-10-11-12-13-15-20(14-4-2)27-23(26)19-16-17-21
InchiKey:	WBMSTNKQTAWCEJ-UHFFFAOYSA-N
Formula:	C23H36F2O2
SMILES:	CCCCCCCCCCCC(CCC)OC(=O)c1ccc(F)c(F)c1
Mol. weight [g/mol]:	382.53

Physical Properties

Property code	Value	Unit	Source
gf	-390.05	kJ/mol	Joback Method
hf	-946.76	kJ/mol	Joback Method
hfus	54.01	kJ/mol	Joback Method
hvap	77.53	kJ/mol	Joback Method
log10ws	-8.77		Crippen Method
logp	7.601		Crippen Method
mvol	322.150	ml/mol	McGowan Method
pc	1000.81	kPa	Joback Method
rinpol	2405.00		NIST Webbook
rinpol	2405.00		NIST Webbook
tb	836.67	K	Joback Method
tc	1027.18	K	Joback Method
tf	458.77	K	Joback Method
vc	1.270	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1020.97	J/mol×K	836.67	Joback Method
cpg	1039.23	J/mol×K	868.42	Joback Method
cpg	1056.38	J/mol×K	900.17	Joback Method
cpg	1072.47	J/mol×K	931.93	Joback Method
cpg	1087.52	J/mol×K	963.68	Joback Method
cpg	1101.57	J/mol×K	995.43	Joback Method
cpg	1114.66	J/mol×K	1027.18	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=U338616&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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