

2,6-Difluoro-3-methylbenzoic acid, 5-tridecyl ester

Inchi:	InChI=1S/C21H32F2O2/c1-4-6-8-9-10-11-13-17(12-7-5-2)25-21(24)19-18(22)15-14-16(3)
InchiKey:	LTECWNDQDDSPNM-UHFFFAOYSA-N
Formula:	C21H32F2O2
SMILES:	CCCCCCCCC(CCCC)OC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]:	354.47

Physical Properties

Property code	Value	Unit	Source
gf	-416.52	kJ/mol	Joback Method
hf	-916.95	kJ/mol	Joback Method
hfus	48.44	kJ/mol	Joback Method
hvap	73.74	kJ/mol	Joback Method
log10ws	-7.99		Crippen Method
logp	6.739		Crippen Method
mcvol	293.970	ml/mol	McGowan Method
pc	1123.06	kPa	Joback Method
rinpol	2279.00		NIST Webbook
rinpol	2279.00		NIST Webbook
tb	795.89	K	Joback Method
tc	982.92	K	Joback Method
tf	448.75	K	Joback Method
vc	1.157	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	900.22	J/molxK	795.89	Joback Method
cpg	917.73	J/molxK	827.06	Joback Method
cpg	934.23	J/molxK	858.23	Joback Method
cpg	949.75	J/molxK	889.41	Joback Method
cpg	964.32	J/molxK	920.58	Joback Method
cpg	977.96	J/molxK	951.75	Joback Method
cpg	990.69	J/molxK	982.92	Joback Method

Sources

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=U338584&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

Latest version available from:

<https://www.chemeo.com/cid/118-470-9/2-6-Difluoro-3-methylbenzoic-acid-5-tridecyl-ester.pdf>

Generated by Cheméo on 2024-05-06 20:09:43.7171179 +0000 UTC m=+17315432.637695222.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.