

Benzamide, 2,6-difluoro-3-methyl-N-octadecyl-

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C26H43F2NO/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-21-29-26(30)24-2

RDLOSUDQIDNRPI-UHFFFAOYSA-N

C26H43F2NO

CCCCCCCCCCCCCCCCCNC(=O)c1c(F)ccc(C)c1F

423.62

Physical Properties

Property code	Value	Unit	Source
gf	-177.59	kJ/mol	Joback Method
hf	-829.18	kJ/mol	Joback Method
hfus	68.83	kJ/mol	Joback Method
hvap	89.28	kJ/mol	Joback Method
log10ws	-10.07		Crippen Method
logp	8.265		Crippen Method
mcvol	368.530	ml/mol	McGowan Method
pc	844.07	kPa	Joback Method
rinpol	3197.00		NIST Webbook
tb	938.48	K	Joback Method
tc	1150.26	K	Joback Method
tf	550.53	K	Joback Method
vc	1.460	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1239.99	J/mol×K	938.48	Joback Method
cpg	1259.47	J/mol×K	973.78	Joback Method
cpg	1277.65	J/mol×K	1009.07	Joback Method
cpg	1294.61	J/mol×K	1044.37	Joback Method
cpg	1310.41	J/mol×K	1079.66	Joback Method
cpg	1325.13	J/mol×K	1114.96	Joback Method
cpg	1338.83	J/mol×K	1150.26	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=U407751&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

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