

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

Inchi:	InChI=1S/C20H31F2NO/c1-3-4-5-6-7-8-9-10-11-12-15-23-20(24)18-17(21)14-13-16(2)19
InchiKey:	OZPMCHCXNOXRAH-UHFFFAOYSA-N
Formula:	C20H31F2NO
SMILES:	CCCCCCCCCCCCNC(=O)c1c(F)ccc(C)c1F
Mol. weight [g/mol]:	339.46

Physical Properties

Property code	Value	Unit	Source
gf	-228.11	kJ/mol	Joback Method
hf	-705.34	kJ/mol	Joback Method
hfus	53.29	kJ/mol	Joback Method
hvap	75.92	kJ/mol	Joback Method
log10ws	-7.56		Crippen Method
logp	5.924		Crippen Method
mvol	283.990	ml/mol	McGowan Method
pc	1217.44	kPa	Joback Method
rinpol	2578.00		NIST Webbook
rinpol	2578.00		NIST Webbook
tb	801.20	K	Joback Method
tc	989.26	K	Joback Method
tf	482.91	K	Joback Method
vc	1.125	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	872.23	J/mol×K	801.20	Joback Method
cpg	889.02	J/mol×K	832.54	Joback Method
cpg	904.87	J/mol×K	863.89	Joback Method
cpg	919.80	J/mol×K	895.23	Joback Method
cpg	933.85	J/mol×K	926.57	Joback Method
cpg	947.07	J/mol×K	957.91	Joback Method
cpg	959.48	J/mol×K	989.26	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407748&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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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