

Benzamide, N,N-diheptyl-2,6-difluoro-

Inchi:	InChI=1S/C21H33F2NO/c1-3-5-7-9-11-16-24(17-12-10-8-6-4-2)21(25)20-18(22)14-13-15
InchiKey:	TVSMWNGIRQEUPY-UHFFFAOYSA-N
Formula:	C21H33F2NO
SMILES:	CCCCCCCN(CCCCCC)C(=O)c1c(F)cccc1F
Mol. weight [g/mol]:	353.49

Physical Properties

Property code	Value	Unit	Source
gf	-188.67	kJ/mol	Joback Method
hf	-700.45	kJ/mol	Joback Method
hfus	54.19	kJ/mol	Joback Method
hvap	73.09	kJ/mol	Joback Method
log10ws	-7.30		Crippen Method
logp	6.348		Crippen Method
mcvol	298.080	ml/mol	McGowan Method
pc	1139.80	kPa	Joback Method
rinpola	2268.00		NIST Webbook
rinpola	2268.00		NIST Webbook
tb	781.37	K	Joback Method
tc	964.73	K	Joback Method
tf	461.47	K	Joback Method
vc	1.163	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	911.58	J/molxK	781.37	Joback Method
cpg	929.42	J/molxK	811.93	Joback Method
cpg	946.28	J/molxK	842.49	Joback Method
cpg	962.21	J/molxK	873.05	Joback Method
cpg	977.25	J/molxK	903.61	Joback Method
cpg	991.44	J/molxK	934.17	Joback Method
cpg	1004.82	J/molxK	964.73	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U308668&Units=SI

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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