

Benzamide, N,N-dinonyl-2,6-difluoro-

Inchi:	InChI=1S/C25H41F2NO/c1-3-5-7-9-11-13-15-20-28(21-16-14-12-10-8-6-4-2)25(29)24-22
InchiKey:	QOSSKJQZZSPXTR-UHFFFAOYSA-N
Formula:	C25H41F2NO
SMILES:	CCCCCCCCCN(CCCCCCCC)C(=O)c1c(F)cccc1F
Mol. weight [g/mol]:	409.60

Physical Properties

Property code	Value	Unit	Source
gf	-154.99	kJ/mol	Joback Method
hf	-783.01	kJ/mol	Joback Method
hfus	64.55	kJ/mol	Joback Method
hvap	82.00	kJ/mol	Joback Method
log10ws	-8.98		Crippen Method
logp	7.908		Crippen Method
mcvol	354.440	ml/mol	McGowan Method
pc	893.20	kPa	Joback Method
rinpol	2656.00		NIST Webbook
rinpol	2656.00		NIST Webbook
tb	872.89	K	Joback Method
tc	1068.73	K	Joback Method
tf	506.55	K	Joback Method
vc	1.387	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1156.05	J/mol×K	872.89	Joback Method
cpg	1175.54	J/mol×K	905.53	Joback Method
cpg	1193.88	J/mol×K	938.17	Joback Method
cpg	1211.13	J/mol×K	970.81	Joback Method
cpg	1227.35	J/mol×K	1003.45	Joback Method
cpg	1242.61	J/mol×K	1036.09	Joback Method
cpg	1256.97	J/mol×K	1068.73	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U308671&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
rlnol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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