

Benzamide, 2,5-difluoro-N-(2,5-difluorobenzoyl)-N-octyl-

Inchi: InChI=1S/C22H23F4NO2/c1-2-3-4-5-6-7-12-27(21(28)17-13-15(23)8-10-19(17)25)22(29)

InchiKey: RKYBGHVJSSSSAB-UHFFFAOYSA-N

Formula: C22H23F4NO2

SMILES: CCCCCCCN(C(=O)c1cc(F)ccc1F)C(=O)c1cc(F)ccc1F

Mol. weight [g/mol]: 409.42

Physical Properties

Property code	Value	Unit	Source
gf	-605.64	kJ/mol	Joback Method
hf	-1012.30	kJ/mol	Joback Method
hfus	57.80	kJ/mol	Joback Method
hvap	84.03	kJ/mol	Joback Method
log10ws	-7.84		Crippen Method
logp	5.886		Crippen Method
mcvol	293.520	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	2433.00		NIST Webbook
rinpol	2433.00		NIST Webbook
tb	893.30	K	Joback Method
tc	1099.13	K	Joback Method
tf	575.31	K	Joback Method
vc	1.153	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	909.86	J/molxK	893.30	Joback Method
cpg	923.64	J/molxK	927.60	Joback Method
cpg	936.41	J/molxK	961.91	Joback Method
cpg	948.22	J/molxK	996.21	Joback Method
cpg	959.14	J/molxK	1030.52	Joback Method
cpg	969.22	J/molxK	1064.82	Joback Method
cpg	978.53	J/molxK	1099.13	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407609&Units=SI
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

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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