Benzamide, 2,5-difluoro-N-(2,5-difluorobenzoyl)-N-(hept-2-yl)-

Inchi: InChI=1S/C21H21F4NO2/c1-3-4-5-6-13(2)26(20(27)16-11-14(22)7-9-18(16)24)21(28)17-

InchiKey: PBLWKOABHIXGAD-UHFFFAOYSA-N

Formula: C21H21F4NO2

SMILES: CCCCCC(C)N(C(=O)c1cc(F)ccc1F)C(=O)c1cc(F)ccc1F

Mol. weight [g/mol]: 395.39

Physical Properties

Property code	Value	Unit	Source
gf	-616.50	kJ/mol	Joback Method
hf	-996.94	kJ/mol	Joback Method
hfus	51.69	kJ/mol	Joback Method
hvap	81.42	kJ/mol	Joback Method
log10ws	-7.53		Crippen Method
logp	5.494		Crippen Method
mcvol	279.430	ml/mol	McGowan Method
pc	1392.29	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tb	869.98	K	Joback Method
tc	1075.77	K	Joback Method
tf	549.04	K	Joback Method
vc	1.091	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	852.20	J/mol×K	869.98	Joback Method
cpg	865.76	J/mol×K	904.28	Joback Method
cpg	878.30	J/mol×K	938.58	Joback Method
cpg	889.89	J/mol×K	972.87	Joback Method
cpg	900.58	J/mol×K	1007.17	Joback Method
cpg	910.43	J/mol×K	1041.47	Joback Method
cpg	919.49	J/mol×K	1075.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407605&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
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