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

Inchi: InChI=1S/C30H39F4NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-20-35(29(36)25-21-23(3

InchiKey: KVWDDAMYWZJBTD-UHFFFAOYSA-N

Formula: C30H39F4NO2

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

Mol. weight [g/mol]: 521.63

Physical Properties

Property code	Value	Unit	Source
gf	-538.28	kJ/mol	Joback Method
hf	-1177.42	kJ/mol	Joback Method
hfus	78.52	kJ/mol	Joback Method
hvap	101.84	kJ/mol	Joback Method
log10ws	-11.19		Crippen Method
logp	9.007		Crippen Method
mcvol	406.240	ml/mol	McGowan Method
pc	792.60	kPa	Joback Method
rinpol	3253.00		NIST Webbook
rinpol	3253.00		NIST Webbook
tb	1076.34	K	Joback Method
tc	1330.18	K	Joback Method
tf	665.47	K	Joback Method
vc	1.601	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1397.71	J/mol×K	1076.34	Joback Method
cpg	1415.08	J/mol×K	1118.65	Joback Method
cpg	1430.99	J/mol×K	1160.95	Joback Method
cpg	1445.61	J/mol×K	1203.26	Joback Method
cpg	1459.08	J/mol×K	1245.57	Joback Method
cpg	1471.57	J/mol×K	1287.87	Joback Method
cpg	1483.21	J/mol×K	1330.18	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407615&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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