Benzamide, N-heptyl-N-octyl-2,6-difluoro-

Inchi: InChI=1S/C22H35F2NO/c1-3-5-7-9-11-13-18-25(17-12-10-8-6-4-2)22(26)21-19(23)15-14
InchiKey: QAPFWRDMYOCOHE-UHFFFAOYSA-N
Formula: C22H35F2NO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)c1c(F)cccc1F
Mol. weight [g/mol]: 367.52

Physical Properties

Property code	Value	Unit	Source
gf	-180.25	kJ/mol	Joback Method
hf	-721.09	kJ/mol	Joback Method
hfus	56.78	kJ/mol	Joback Method
hvap	75.32	kJ/mol	Joback Method
log10ws	-7.72		Crippen Method
logp	6.738		Crippen Method
mcvol	312.170	ml/mol	McGowan Method
pc	1069.36	kPa	Joback Method
rinpol	2369.00		NIST Webbook
rinpol	2369.00		NIST Webbook
tb	804.25	K	Joback Method
tc	989.59	K	Joback Method
tf	472.74	K	Joback Method
vc	1.220	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	971.53	J/mol×K	804.25	Joback Method
cpg	989.73	J/mol×K	835.14	Joback Method
cpg	1006.92	J/mol×K	866.03	Joback Method
cpg	1023.15	J/mol×K	896.92	Joback Method
cpg	1038.46	J/mol×K	927.81	Joback Method
cpg	1052.89	J/mol×K	958.70	Joback Method
cpg	1066.50	J/mol×K	989.59	Joback Method

Sources

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=U308669&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

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