

Benzamide, N-heptyl-N-octyl-3-fluoro-

Inchi:	InChI=1S/C22H36FNO/c1-3-5-7-9-11-13-18-24(17-12-10-8-6-4-2)22(25)20-15-14-16-21(
InchiKey:	PIIHEAYJPNUCQP-UHFFFAOYSA-N
Formula:	C22H36FNO
SMILES:	CCCCCCCCN(CCCCCC)C(=O)c1cccc(F)c1
Mol. weight [g/mol]:	349.53

Physical Properties

Property code	Value	Unit	Source
gf	24.19	kJ/mol	Joback Method
hf	-513.51	kJ/mol	Joback Method
hfus	54.09	kJ/mol	Joback Method
hvap	75.48	kJ/mol	Joback Method
log10ws	-7.39		Crippen Method
logp	6.599		Crippen Method
mvol	310.400	ml/mol	McGowan Method
pc	1112.59	kPa	Joback Method
rinpol	2432.00		NIST Webbook
rinpol	2432.00		NIST Webbook
tb	800.00	K	Joback Method
tc	987.39	K	Joback Method
tf	459.63	K	Joback Method
vc	1.202	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.18	J/molxK	800.00	Joback Method
cpg	982.84	J/molxK	831.23	Joback Method
cpg	1000.45	J/molxK	862.46	Joback Method
cpg	1017.07	J/molxK	893.70	Joback Method
cpg	1032.75	J/molxK	924.93	Joback Method
cpg	1047.53	J/molxK	956.16	Joback Method
cpg	1061.48	J/molxK	987.39	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U308400&Units=SI

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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