Benzamide, n-heptyl-n-octyl-4-fluoro-

Inchi: InChI=1S/C22H36FNO/c1-3-5-7-9-11-13-19-24(18-12-10-8-6-4-2)22(25)20-14-16-21(23)
InchiKey: BSMHNSMJYSIEIP-UHFFFAOYSA-N
Formula: C22H36FNO
SMILES: CCCCCCCCN(CCCCCCC)C(=O)c1ccc(F)cc1
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
mcvol	310.400	ml/mol	McGowan Method
pc	1112.59	kPa	Joback Method
rinpol	2441.00		NIST Webbook
rinpol	2441.00		NIST Webbook
tb	800.00	K	Joback Method
tc	987.39	K	Joback Method
tf	459.63	K	Joback Method
vc	1.202	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	964.18	J/mol×K	800.00	Joback Method
cpg	982.84	J/mol×K	831.23	Joback Method
cpg	1000.45	J/mol×K	862.46	Joback Method
cpg	1017.07	J/mol×K	893.70	Joback Method
cpg	1032.75	J/mol×K	924.93	Joback Method
cpg	1047.53	J/mol×K	956.16	Joback Method
cpg	1061.48	J/mol×K	987.39	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=U308309&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