Benzamide, 2-fluoro-3-trifluoromethyl-N-pentyl-N-octyl-

Inchi: InChI=1S/C21H31F4NO/c1-3-5-7-8-9-11-16-26(15-10-6-4-2)20(27)17-13-12-14-18(19(17

InchiKey: ZCGJJMNRMGBSCK-UHFFFAOYSA-N

Formula: C21H31F4NO

SMILES: CCCCCCCCN(CCCCC)C(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 389.47

Physical Properties

Property code	Value	Unit	Source
gf	-575.45	kJ/mol	Joback Method
hf	-1101.42	kJ/mol	Joback Method
hfus	52.93	kJ/mol	Joback Method
hvap	70.17	kJ/mol	Joback Method
log10ws	-7.66		Crippen Method
logp	6.837		Crippen Method
mcvol	301.620	ml/mol	McGowan Method
pc	1087.06	kPa	Joback Method
rinpol	2746.00		NIST Webbook
rinpol	2746.00		NIST Webbook
tb	776.68	K	Joback Method
tc	957.10	K	Joback Method
tf	465.07	K	Joback Method
vc	1.188	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	928.01	J/mol×K	776.68	Joback Method
cpg	945.17	J/mol×K	806.75	Joback Method
cpg	961.38	J/mol×K	836.82	Joback Method
cpg	976.67	J/mol×K	866.89	Joback Method
cpg	991.12	J/mol×K	896.96	Joback Method
cpg	1004.77	J/mol×K	927.03	Joback Method
cpg	1017.69	J/mol×K	957.10	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=U416696&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