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

Inchi: InChI=1S/C23H35F4NO/c1-3-5-7-8-9-10-11-13-18-28(17-12-6-4-2)22(29)19-15-14-16-20

InchiKey: PNUKYXIDTGVUJO-UHFFFAOYSA-N

Formula: C23H35F4NO

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

Mol. weight [g/mol]: 417.52

Physical Properties

Property code	Value	Unit	Source
gf	-558.61	kJ/mol	Joback Method
hf	-1142.70	kJ/mol	Joback Method
hfus	58.12	kJ/mol	Joback Method
hvap	74.62	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	7.618		Crippen Method
mcvol	329.800	ml/mol	McGowan Method
pc	961.48	kPa	Joback Method
rinpol	2987.00		NIST Webbook
rinpol	2987.00		NIST Webbook
tb	822.44	K	Joback Method
tc	1008.42	K	Joback Method
tf	487.61	K	Joback Method
vc	1.300	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1047.84	J/mol×K	822.44	Joback Method
cpg	1065.82	J/mol×K	853.44	Joback Method
cpg	1082.79	J/mol×K	884.43	Joback Method
cpg	1098.79	J/mol×K	915.43	Joback Method
cpg	1113.91	J/mol×K	946.43	Joback Method
cpg	1128.19	J/mol×K	977.42	Joback Method
cpg	1141.71	J/mol×K	1008.42	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=U416698&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
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