Benzamide, 3-fluoro-4-trifluoromethyl-N-hexadecyl-

Inchi: InChI=1S/C24H37F4NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-18-29-23(30)20-16-17-21

InchiKey: TVHQSYRZAJPHOD-UHFFFAOYSA-N

Formula: C24H37F4NO

SMILES: CCCCCCCCCCCCCCCCCNC(=O)c1ccc(C(F)(F)F)c(F)c1

Mol. weight [g/mol]: 431.55

Physical Properties

Property code	Value	Unit	Source
gf	-571.58	kJ/mol	Joback Method
hf	-1177.40	kJ/mol	Joback Method
hfus	62.78	kJ/mol	Joback Method
hvap	81.24	kJ/mol	Joback Method
log10ws	-9.53		Crippen Method
logp	8.056		Crippen Method
mcvol	343.890	ml/mol	McGowan Method
pc	914.94	kPa	Joback Method
rinpol	2802.00		NIST Webbook
rinpol	2802.00		NIST Webbook
tb	883.05	K	Joback Method
tc	1081.10	K	Joback Method
tf	519.07	K	Joback Method
vc	1.373	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1129.53	J/mol×K	883.05	Joback Method
cpg	1147.52	J/mol×K	916.06	Joback Method
cpg	1164.42	J/mol×K	949.07	Joback Method
cpg	1180.33	J/mol×K	982.08	Joback Method
cpg	1195.30	J/mol×K	1015.09	Joback Method
cpg	1209.41	J/mol×K	1048.09	Joback Method
cpg	1222.74	J/mol×K	1081.10	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407899&Units=SI
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

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