Benzamide, 3-trifluoromethyl-2-fluoro-N-tetradecyl-

Inchi: InChI=1S/C22H33F4NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-17-27-21(28)18-15-14-16-19(20

InchiKey: CZMQCOFCCBFNNQ-UHFFFAOYSA-N

Formula: C22H33F4NO

SMILES: CCCCCCCCCCCCCCNC(=O)c1cccc(C(F)(F)F)c1F

Mol. weight [g/mol]: 403.50

Physical Properties

Property code	Value	Unit	Source
gf	-588.42	kJ/mol	Joback Method
hf	-1136.12	kJ/mol	Joback Method
hfus	57.60	kJ/mol	Joback Method
hvap	76.78	kJ/mol	Joback Method
log10ws	-8.69		Crippen Method
logp	7.275		Crippen Method
mcvol	315.710	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinpol	2537.00		NIST Webbook
rinpol	2537.00		NIST Webbook
tb	837.29	K	Joback Method
tc	1026.76	K	Joback Method
tf	496.53	K	Joback Method
vc	1.262	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1007.71	J/mol×K	837.29	Joback Method
cpg	1024.71	J/mol×K	868.87	Joback Method
cpg	1040.72	J/mol×K	900.45	Joback Method
cpg	1055.80	J/mol×K	932.03	Joback Method
cpg	1070.01	J/mol×K	963.60	Joback Method
cpg	1083.41	J/mol×K	995.18	Joback Method
cpg	1096.05	J/mol×K	1026.76	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=U407713&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