Benzamide, 2,5-di(trifluoromethyl)-N-tetradecyl-

Inchi: InChI=1S/C23H33F6NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-30-21(31)19-17-18(22(24,25

InchiKey: VIQAUWIXPXXIJZ-UHFFFAOYSA-N

Formula: C23H33F6NO

SMILES: CCCCCCCCCCCCCCNC(=O)c1cc(C(F)(F)F)ccc1C(F)(F)F

Mol. weight [g/mol]: 453.50

Physical Properties

Property code	Value	Unit	Source
gf	-966.78	kJ/mol	Joback Method
hf	-1557.73	kJ/mol	Joback Method
hfus	58.94	kJ/mol	Joback Method
hvap	76.08	kJ/mol	Joback Method
log10ws	-9.47		Crippen Method
logp	8.155		Crippen Method
mcvol	333.340	ml/mol	McGowan Method
pc	928.94	kPa	Joback Method
rinpol	2432.00		NIST Webbook
rinpol	2432.00		NIST Webbook
tb	855.48	K	Joback Method
tc	1047.42	K	Joback Method
tf	511.40	K	Joback Method
vc	1.343	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1083.44	J/mol×K	855.48	Joback Method
cpg	1100.37	J/mol×K	887.47	Joback Method
cpg	1116.31	J/mol×K	919.46	Joback Method
cpg	1131.34	J/mol×K	951.45	Joback Method
cpg	1145.53	J/mol×K	983.44	Joback Method
cpg	1158.98	J/mol×K	1015.43	Joback Method
cpg	1171.76	J/mol×K	1047.42	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=U407930&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