Benzamide, 2,3,4-trifluoro-N-butyl-N-tetradecyl-

Inchi: InChI=1S/C25H40F3NO/c1-3-5-7-8-9-10-11-12-13-14-15-16-20-29(19-6-4-2)25(30)21-17

InchiKey: KDIXDTGIMIFDPR-UHFFFAOYSA-N

Formula: C25H40F3NO

SMILES: CCCCCCCCCCCCCCN(CCCC)C(=O)c1ccc(F)c(F)c1F

Mol. weight [g/mol]: 427.59

Physical Properties

Property code	Value	Unit	Source
gf	-359.43	kJ/mol	Joback Method
hf	-990.59	kJ/mol	Joback Method
hfus	67.24	kJ/mol	Joback Method
hvap	81.84	kJ/mol	Joback Method
log10ws	-9.31		Crippen Method
logp	8.047		Crippen Method
mcvol	356.210	ml/mol	McGowan Method
pc	862.01	kPa	Joback Method
rinpol	3361.00		NIST Webbook
rinpol	3361.00		NIST Webbook
tb	877.14	K	Joback Method
tc	1073.99	K	Joback Method
tf	519.66	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1163.14	J/mol×K	877.14	Joback Method
cpg	1182.47	J/mol×K	909.95	Joback Method
cpg	1200.63	J/mol×K	942.76	Joback Method
cpg	1217.69	J/mol×K	975.57	Joback Method
cpg	1233.71	J/mol×K	1008.38	Joback Method
cpg	1248.75	J/mol×K	1041.19	Joback Method
cpg	1262.87	J/mol×K	1073.99	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415690&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

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