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

Inchi: InChI=1S/C23H36F3NO/c1-3-5-7-8-9-10-11-12-13-14-18-27(17-6-4-2)23(28)19-15-16-20
InchiKey: UWUWEDRDSBNQQE-UHFFFAOYSA-N
Formula: C23H36F3NO
SMILES: CCCCCCCCCCCCN(CCCC)C(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 399.53

Physical Properties

Property code	Value	Unit	Source
gf	-376.27	kJ/mol	Joback Method
hf	-949.31	kJ/mol	Joback Method
hfus	62.06	kJ/mol	Joback Method
hvap	77.39	kJ/mol	Joback Method
log10ws	-8.47		Crippen Method
logp	7.267		Crippen Method
mcvol	328.030	ml/mol	McGowan Method
pc	968.07	kPa	Joback Method
rinpol	3266.00		NIST Webbook
rinpol	3266.00		NIST Webbook
tb	831.38	K	Joback Method
tc	1018.81	K	Joback Method
tf	497.12	K	Joback Method
vc	1.294	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1039.53	J/mol×K	831.38	Joback Method
cpg	1057.81	J/mol×K	862.62	Joback Method
cpg	1075.05	J/mol×K	893.86	Joback Method
cpg	1091.31	J/mol×K	925.10	Joback Method
cpg	1106.62	J/mol×K	956.34	Joback Method
cpg	1121.04	J/mol×K	987.57	Joback Method
cpg	1134.61	J/mol×K	1018.81	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415689&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

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