Benzamide, 3-trifluoromethyl-N-ethyl-N-dodecyl-

Inchi: InChI=1S/C22H34F3NO/c1-3-5-6-7-8-9-10-11-12-13-17-26(4-2)21(27)19-15-14-16-20(18

InchiKey: OKZFYYKQZYZLLN-UHFFFAOYSA-N

Formula: C22H34F3NO

SMILES: CCCCCCCCCCCCN(CC)C(=O)c1cccc(C(F)(F)F)c1

Mol. weight [g/mol]: 385.51

Physical Properties

Property code	Value	Unit	Source
gf	-362.59	kJ/mol	Joback Method
hf	-914.48	kJ/mol	Joback Method
hfus	52.83	kJ/mol	Joback Method
hvap	72.55	kJ/mol	Joback Method
log10ws	-7.74		Crippen Method
logp	7.088		Crippen Method
mcvol	313.940	ml/mol	McGowan Method
pc	1061.71	kPa	Joback Method
rinpol	2766.00		NIST Webbook
rinpol	2766.00		NIST Webbook
tb	795.31	K	Joback Method
tc	979.76	K	Joback Method
tf	463.23	K	Joback Method
vc	1.226	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	980.21	J/mol×K	795.31	Joback Method
cpg	998.17	J/mol×K	826.05	Joback Method
cpg	1015.12	J/mol×K	856.79	Joback Method
cpg	1031.11	J/mol×K	887.54	Joback Method
cpg	1046.20	J/mol×K	918.28	Joback Method
cpg	1060.48	J/mol×K	949.02	Joback Method
cpg	1073.98	J/mol×K	979.76	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=U415581&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