Benzamide, 4-(trifluoromethyl)-N-tetradecyl-

Inchi: InChI=1S/C22H34F3NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-18-26-21(27)19-14-16-20(17-15
InchiKey: POBUNAJREPPJCW-UHFFFAOYSA-N
Formula: C22H34F3NO
SMILES: CCCCCCCCCCCCCCNC(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 385.51

Physical Properties

Property code	Value	Unit	Source
gf	-383.98	kJ/mol	Joback Method
hf	-928.54	kJ/mol	Joback Method
hfus	54.91	kJ/mol	Joback Method
hvap	76.94	kJ/mol	Joback Method
log10ws	-8.36		Crippen Method
logp	7.136		Crippen Method
mcvol	313.940	ml/mol	McGowan Method
pc	1072.17	kPa	Joback Method
rinpol	2629.00		NIST Webbook
rinpol	2629.00		NIST Webbook
tb	833.04	K	Joback Method
tc	1023.50	K	Joback Method
tf	483.42	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1000.70	J/mol×K	833.04	Joback Method
cpg	1018.04	J/mol×K	864.78	Joback Method
cpg	1034.37	J/mol×K	896.53	Joback Method
cpg	1049.75	J/mol×K	928.27	Joback Method
cpg	1064.24	J/mol×K	960.01	Joback Method
cpg	1077.93	J/mol×K	991.76	Joback Method
cpg	1090.86	J/mol×K	1023.50	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=U407309&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