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

Inchi: InChI=1S/C21H32F3NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-16-25-21(26)17-14-15-18(22)20
InchiKey: QYRBCIBBXDLNQE-UHFFFAOYSA-N
Formula: C21H32F3NO
SMILES: CCCCCCCCCCCCCCNC(=O)c1ccc(F)c(F)c1F
Mol. weight [g/mol]: 371.48

Physical Properties

Property code	Value	Unit	Source
gf	-414.50	kJ/mol	Joback Method
hf	-922.09	kJ/mol	Joback Method
hfus	58.96	kJ/mol	Joback Method
hvap	77.33	kJ/mol	Joback Method
log10ws	-8.25		Crippen Method
logp	6.535		Crippen Method
mcvol	299.850	ml/mol	McGowan Method
pc	1105.94	kPa	Joback Method
rinpol	2554.00		NIST Webbook
rinpol	2554.00		NIST Webbook
tb	823.35	K	Joback Method
tc	1010.90	K	Joback Method
tf	494.77	K	Joback Method
vc	1.198	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	939.07	J/mol×K	823.35	Joback Method
cpg	955.92	J/mol×K	854.61	Joback Method
cpg	971.81	J/mol×K	885.87	Joback Method
cpg	986.77	J/mol×K	917.12	Joback Method
cpg	1000.83	J/mol×K	948.38	Joback Method
cpg	1014.05	J/mol×K	979.64	Joback Method
cpg	1026.45	J/mol×K	1010.90	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=U407271&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