Benzamide, 4-(trifluoromethyl)-N-butyl-N-hexadecyl-

Inchi: InChI=1S/C28H46F3NO/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-24-32(23-6-4-2)27(33
InchiKey: FUKVYCLOLQMYJI-UHFFFAOYSA-N
Formula: C28H46F3NO
SMILES: CCCCCCCCCCCCCCCCN(CCCC)C(=O)c1ccc(C(F)(F)F)cc1
Mol. weight [g/mol]: 469.67

Physical Properties

Property code	Value	Unit	Source
gf	-312.07	kJ/mol	Joback Method
hf	-1038.32	kJ/mol	Joback Method
hfus	68.37	kJ/mol	Joback Method
hvap	85.90	kJ/mol	Joback Method
log10ws	-10.25		Crippen Method
logp	9.429		Crippen Method
mcvol	398.480	ml/mol	McGowan Method
pc	752.67	kPa	Joback Method
rinpol	2410.00		NIST Webbook
rinpol	2410.00		NIST Webbook
tb	932.59	K	Joback Method
tc	1144.25	K	Joback Method
tf	530.85	K	Joback Method
vc	1.562	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1353.10	J/mol×K	932.59	Joback Method
cpg	1374.05	J/mol×K	967.87	Joback Method
cpg	1393.74	J/mol×K	1003.14	Joback Method
cpg	1412.31	J/mol×K	1038.42	Joback Method
cpg	1429.85	J/mol×K	1073.69	Joback Method
cpg	1446.50	J/mol×K	1108.97	Joback Method
cpg	1462.35	J/mol×K	1144.25	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=U415710&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