Benzamide, 3-(trifluoromethyl)-N-hexadecyl-

Inchi: InChI=1S/C24H38F3NO/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-19-28-23(29)21-17-16-18
InchiKey: JQUMXNPZURYTDN-UHFFFAOYSA-N
Formula: C24H38F3NO
SMILES: CCCCCCCCCCCCCCCCCNC(=O)c1cccc(C(F)(F)F)c1
Mol. weight [g/mol]: 413.56

Physical Properties

Property code	Value	Unit	Source
gf	-367.14	kJ/mol	Joback Method
hf	-969.82	kJ/mol	Joback Method
hfus	60.09	kJ/mol	Joback Method
hvap	81.39	kJ/mol	Joback Method
log10ws	-9.20		Crippen Method
logp	7.917		Crippen Method
mcvol	342.120	ml/mol	McGowan Method
pc	949.08	kPa	Joback Method
rinpol	2814.00		NIST Webbook
rinpol	2814.00		NIST Webbook
tb	878.80	K	Joback Method
tc	1076.24	K	Joback Method
tf	505.96	K	Joback Method
vc	1.355	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1122.65	J/mol×K	878.80	Joback Method
cpg	1140.84	J/mol×K	911.71	Joback Method
cpg	1157.95	J/mol×K	944.61	Joback Method
cpg	1174.06	J/mol×K	977.52	Joback Method
cpg	1189.25	J/mol×K	1010.42	Joback Method
cpg	1203.59	J/mol×K	1043.33	Joback Method
cpg	1217.17	J/mol×K	1076.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U407180&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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