

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

Inchi: InChI=1S/C19H28F3NO/c1-3-5-7-8-9-15-23(14-6-4-2)18(24)16-10-12-17(13-11-16)19(20)

InchiKey: LOEIQYNQBHCDGS-UHFFFAOYSA-N

Formula: C19H28F3NO

SMILES: CCCCCCN(CCCC)C(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 343.43

Physical Properties

Property code	Value	Unit	Source
gf	-387.85	kJ/mol	Joback Method
hf	-852.56	kJ/mol	Joback Method
hfus	45.06	kJ/mol	Joback Method
hvap	65.87	kJ/mol	Joback Method
log10ws	-6.49		Crippen Method
logp	5.918		Crippen Method
mvol	271.670	ml/mol	McGowan Method
pc	1293.00	kPa	Joback Method
rinpol	2636.00		NIST Webbook
rinpol	2636.00		NIST Webbook
tb	726.67	K	Joback Method
tc	907.83	K	Joback Method
tf	429.42	K	Joback Method
vc	1.058	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.19	J/mol×K	726.67	Joback Method
cpg	821.24	J/mol×K	756.86	Joback Method
cpg	837.31	J/mol×K	787.06	Joback Method
cpg	852.46	J/mol×K	817.25	Joback Method
cpg	866.75	J/mol×K	847.44	Joback Method
cpg	880.23	J/mol×K	877.64	Joback Method
cpg	892.96	J/mol×K	907.83	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U415703&Units=SI

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
hvpap:	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
rinppl:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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