Benzamide, 4-(trifluoromethyl)-N-butyl-N-2-ethylhexyl-

Inchi: InChI=1S/C20H30F3NO/c1-4-7-9-16(6-3)15-24(14-8-5-2)19(25)17-10-12-18(13-11-17)20

InchiKey: NBSJRCSDEMTBFG-UHFFFAOYSA-N

Formula: C20H30F3NO

SMILES: CCCCC(CC)CN(CCCC)C(=O)c1ccc(C(F)(F)F)cc1

Mol. weight [g/mol]: 357.45

Physical Properties

Property code	Value	Unit	Source
gf	-381.87	kJ/mol	Joback Method
hf	-878.48	kJ/mol	Joback Method
hfus	44.13	kJ/mol	Joback Method
hvap	67.71	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	6.164		Crippen Method
mcvol	285.760	ml/mol	McGowan Method
pc	1214.90	kPa	Joback Method
rinpol	2475.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	749.11	K	Joback Method
tc	932.56	K	Joback Method
tf	425.69	K	Joback Method
vc	1.109	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	862.43	J/mol×K	749.11	Joback Method
cpg	879.95	J/mol×K	779.69	Joback Method
cpg	896.46	J/mol×K	810.26	Joback Method
cpg	912.01	J/mol×K	840.84	Joback Method
cpg	926.67	J/mol×K	871.41	Joback Method
cpg	940.49	J/mol×K	901.99	Joback Method
cpg	953.53	J/mol×K	932.56	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415702&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