Phenethylamine, n,n-dibutyl-

Other names: N,N-dibutylphenethylamine
Inchi: InChI=1S/C16H27N/c1-3-5-13-17(14-6-4-2)15-12-16-10-8-7-9-11-16/h7-11H,3-6,12-15H2
InchiKey: LEHSOUZQZPUDEC-UHFFFAOYSA-N
Formula: C16H27N
SMILES: CCCCN(CCCC)CCc1ccccc1
Mol. weight [g/mol]: 233.39
CAS: 5779-51-1

Physical Properties

Property code	Value	Unit	Source
gf	307.03	kJ/mol	Joback Method
hf	-69.51	kJ/mol	Joback Method
hfus	34.26	kJ/mol	Joback Method
hvap	55.53	kJ/mol	Joback Method
log10ws	-4.19		Crippen Method
logp	4.131		Crippen Method
mcvol	222.520	ml/mol	McGowan Method
pc	1700.50	kPa	Joback Method
tb	604.60	K	Joback Method
tc	791.89	K	Joback Method
tf	328.97	K	Joback Method
vc	0.842	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	583.74	J/mol×K	604.60	Joback Method
cpg	603.09	J/mol×K	635.81	Joback Method
cpg	621.40	J/mol×K	667.03	Joback Method
cpg	638.73	J/mol×K	698.24	Joback Method
cpg	655.12	J/mol×K	729.46	Joback Method
cpg	670.61	J/mol×K	760.67	Joback Method
cpg	685.25	J/mol×K	791.89	Joback Method

Sources

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=C5779511&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume