

Norcamphane, 3-ethylamino-3-phenyl

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C17H25N/c1-4-18-17(13-8-6-5-7-9-13)15-11-10-14(12-15)16(17,2)3/h5-9,14-17

ZYONEPPWRXYDCM-BTPDTDQASA-N

C17H25N

CCNC1(c2ccccc2)C2CCC(C2)C1(C)C

243.39

Physical Properties

Property code	Value	Unit	Source
gf	377.06	kJ/mol	Joback Method
hf	25.03	kJ/mol	Joback Method
hfus	22.64	kJ/mol	Joback Method
hvap	59.23	kJ/mol	Joback Method
log10ws	-4.46		Crippen Method
logp	3.948		Crippen Method
mcvol	214.890	ml/mol	McGowan Method
pc	2071.76	kPa	Joback Method
rinpol	1570.00		NIST Webbook
rinpol	1570.00		NIST Webbook
tb	674.10	K	Joback Method
tc	908.62	K	Joback Method
tf	432.11	K	Joback Method
vc	0.815	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	630.97	J/mol×K	674.10	Joback Method
cpg	652.79	J/mol×K	713.19	Joback Method
cpg	673.62	J/mol×K	752.27	Joback Method
cpg	693.78	J/mol×K	791.36	Joback Method
cpg	713.60	J/mol×K	830.45	Joback Method
cpg	733.43	J/mol×K	869.53	Joback Method
cpg	753.60	J/mol×K	908.62	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R18218&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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