

Etidocaine

Other names:

Butanamide, N-(2,6-dimethylphenyl)-2-(ethylpropylamino)-, (.+/-.)-
N-(2,6-Dimethylphenyl)-2-(ethylpropylamino)butanamide
Duranest

2-(Ethylpropylamino)-2',6'-butyroxylidide
(.+/-.)-2-(Ethylpropylamino)-2',6'-butyroxylidide

Inchi:

InChI=1S/C17H28N2O/c1-6-12-19(8-3)15(7-2)17(20)18-16-13(4)10-9-11-14(16)5/h9-11,1

InchiKey:

VTUSIVBDOCDNHS-UHFFFAOYSA-N

Formula:

C17H28N2O

SMILES:

CCCN(CC)C(CC)C(=O)Nc1c(C)cccc1C

Mol. weight [g/mol]:

276.42

CAS:

36637-18-0

Physical Properties

Property code	Value	Unit	Source
gf	254.22	kJ/mol	Joback Method
hf	-177.48	kJ/mol	Joback Method
hfus	39.24	kJ/mol	Joback Method
hvap	71.87	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	3.752		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
pc	1643.09	kPa	Joback Method
rinpol	2024.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tb	741.04	K	Joback Method
tc	939.75	K	Joback Method
tf	452.87	K	Joback Method
vc	0.932	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	726.02	J/mol×K	741.04	Joback Method
cpg	743.32	J/mol×K	774.16	Joback Method

cpg	759.59	J/mol×K	807.28	Joback Method
cpg	774.88	J/mol×K	840.40	Joback Method
cpg	789.24	J/mol×K	873.51	Joback Method
cpg	802.70	J/mol×K	906.63	Joback Method
cpg	815.32	J/mol×K	939.75	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=C36637180&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
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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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