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

Physical Properties

Property code	Value	Unit	Source
hfus	39.24	kJ/mol	Joback Method
ie	7.19	eV	Cheméo Relay (1.0)
log10ws	-2.62		Cheméo Relay (1.0)
logp	3.752		Crippen Method
mcvol	248.160	ml/mol	McGowan Method
rinpol	2024.00		NIST Webbook
rinpol	2030.00		NIST Webbook
tf	375.65	K	Cheméo Relay (1.0)

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:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36637180&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tf:	Normal melting (fusion) point