Tramadol

Other names:	Ultram
	(.+/-.)-2-[(Dimethylamino)methyl]-1-(3-methoxyphenyl)cyclohexanol, cis-
	CG 315E
	E 265
	U 26255A
	2-[(Dimethylamino)methyl]-1-(3-methoxyphenyl)cyclohexanol, cis-
	(.+/-.)-Tramadol
	Cyclohexanol, 2-((dimethylamino)methyl)-1-(3-methoxyphenyl)-, cis-(.+/-.)-
	Cyclohexanol, 2-((dimethylamino)methyl)-1-(m-methoxyphenyl)-
Inchi:	InChI=1S/C16H25NO2/c1-17(2)12-14-7-4-5-10-16(14,18)13-8-6-9-15(11-13)19-3/h6,8-9,
InchiKey:	TVYLLZQTGLZFBW-UHFFFAOYSA-N
Formula:	C16H25NO2
SMILES:	COc1cccc(C2(O)CCCCC2CN(C)C)c1
Mol. weight [g/mol]:	263.38
CAS:	27203-92-5

Physical Properties

Property code	Value	Unit	Source
gf	66.83	kJ/mol	Joback Method
hf	-316.21	kJ/mol	Joback Method
hfus	25.75	kJ/mol	Joback Method
hvap	74.25	kJ/mol	Joback Method
log10ws	-2.98		Crippen Method
logp	2.635		Crippen Method
mcvol	223.400	ml/mol	McGowan Method
pc	2167.36	kPa	Joback Method
rinpol	1999.00		NIST Webbook
rinpol	1945.00		NIST Webbook
rinpol	1999.00		NIST Webbook
rinpol	1991.30		NIST Webbook
rinpol	1991.30		NIST Webbook
tb	739.30	K	Joback Method
tc	949.64	K	Joback Method
tf	451.58	K	Joback Method
vc	0.808	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	676.71	J/mol×K	739.30	Joback Method
cpg	695.05	J/mol×K	774.36	Joback Method
cpg	712.53	J/mol×K	809.41	Joback Method
cpg	729.26	J/mol×K	844.47	Joback Method
cpg	745.36	J/mol×K	879.52	Joback Method
cpg	760.94	J/mol×K	914.58	Joback Method
cpg	776.13	J/mol×K	949.64	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27203925&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