Crotamiton

Other names:	2-Butenamide, N-ethyl-N-(2-methylphenyl)- o-Crotonotoluidide, N-ethyl- Crotalgin Crotonyl-N-ethyl-o-toluidine Eurax Euraxil N-Ethyl-o-crotonotoluidide Veteusan N-Ethyl-ortho-crotonotoluidide Crotamitone N-Ethyl-o-crotonotoluidine Eurasil Crotamitex
Inchi:	InChI=1S/C13H17NO/c1-4-8-13(15)14(5-2)12-10-7-6-9-11(12)3/h4,6-10H,5H2,1-3H3/b8-
InchiKey:	DNTGGZPQPQTDQF-XBXARRHUSA-N
Formula:	C13H17NO
SMILES:	CC=CC(=O)N(CC)c1ccccc1C
Mol. weight [g/mol]:	203.28
CAS:	483-63-6

Physical Properties

Property code	Value	Unit	Source
gf	223.44	kJ/mol	Joback Method
hf	-14.42	kJ/mol	Joback Method
hfus	27.90	kJ/mol	Joback Method
hvap	56.22	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.924		Crippen Method
mcvol	177.520	ml/mol	McGowan Method
pc	2410.00	kPa	Joback Method
rinpol	1550.00		NIST Webbook
rinpol	1540.00		NIST Webbook
rinpol	1550.00		NIST Webbook
rinpol	1550.00		NIST Webbook
tb	598.97	K	Joback Method
tc	810.67	K	Joback Method
tf	352.53	K	Joback Method

vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	433.69	J/mol×K	598.97	Joback Method
cpg	449.54	J/mol×K	634.25	Joback Method
cpg	464.39	J/mol×K	669.54	Joback Method
cpg	478.28	J/mol×K	704.82	Joback Method
cpg	491.28	J/mol×K	740.11	Joback Method
cpg	503.43	J/mol×K	775.39	Joback Method
cpg	514.80	J/mol×K	810.67	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	427.20	K	1.70	NIST Webbook

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=C483636&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume