

Diethyltoluamide

Other names:	Benzamide, N,N-diethyl-3-methyl- m-Toluamide, N,N-diethyl- m-Delphene m-DETA m-Toluic Acid diethylamide A.I. 3-22542 Autan Delphene Detamide Dieltamid DEET DET DETA ENT 20,218 ENT 22542 Flypel M-DET Metadelphene N,N-Diethyl-m-Toluamide N,N-Diethyl-3-methylbenzamide Naugatuck DET Off Repper-DET Repudin-Special 3-Methyl-N,N-diethylbenzamide Diethyl-m-toluamide DETA-20 AI 3-22542 Chemform MGK diethyltoluamide Repel Amincene C 140 Amincene C-EM DET (insect repellent) NSC 33840
Inchi:	InChI=1S/C12H17NO/c1-4-13(5-2)12(14)11-8-6-7-10(3)9-11/h6-9H,4-5H2,1-3H3
InchiKey:	MMOXZBCLCQITDF-UHFFFAOYSA-N
Formula:	C12H17NO
SMILES:	CCN(CC)C(=O)c1cccc(C)c1
Mol. weight [g/mol]:	191.27

Physical Properties

Property code	Value	Unit	Source
gf	134.80	kJ/mol	Joback Method
hf	-111.00	kJ/mol	Joback Method
hfus	25.11	kJ/mol	Joback Method
hvap	54.03	kJ/mol	Joback Method
log10ws	-2.93		Crippen Method
logp	2.477		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2517.59	kPa	Joback Method
rinpol	1571.00		NIST Webbook
rinpol	1571.00		NIST Webbook
rinpol	269.36		NIST Webbook
rinpol	1583.00		NIST Webbook
rinpol	1571.00		NIST Webbook
tb	571.93	K	Joback Method
tc	778.19	K	Joback Method
tf	346.34	K	Joback Method
vc	0.624	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	404.24	J/mol×K	571.93	Joback Method
cpg	420.02	J/mol×K	606.31	Joback Method
cpg	434.87	J/mol×K	640.68	Joback Method
cpg	448.82	J/mol×K	675.06	Joback Method
cpg	461.92	J/mol×K	709.43	Joback Method
cpg	474.20	J/mol×K	743.81	Joback Method
cpg	485.70	J/mol×K	778.19	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	433.20	K	2.50	NIST Webbook
tbrp	384.20	K	0.10	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C134623&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
rinpola:	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

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