

Octanamide, N-ethyl-N-(3-methylphenyl)-

Inchi:	InChI=1S/C17H27NO/c1-4-6-7-8-9-13-17(19)18(5-2)16-12-10-11-15(3)14-16/h10-12,14H
InchiKey:	RTKPBOCQCMXBJO-UHFFFAOYSA-N
Formula:	C17H27NO
SMILES:	CCCCCCCC(=O)N(CC)c1cccc(C)c1
Mol. weight [g/mol]:	261.40

Physical Properties

Property code	Value	Unit	Source
gf	176.90	kJ/mol	Joback Method
hf	-214.20	kJ/mol	Joback Method
hfus	38.06	kJ/mol	Joback Method
hvap	65.16	kJ/mol	Joback Method
log10ws	-4.98		Crippen Method
logp	4.708		Crippen Method
mvol	238.180	ml/mol	McGowan Method
pc	1635.13	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	1925.00		NIST Webbook
tb	686.33	K	Joback Method
tc	879.80	K	Joback Method
tf	402.69	K	Joback Method
vc	0.903	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.78	J/mol×K	686.33	Joback Method
cpg	683.67	J/mol×K	718.58	Joback Method
cpg	700.55	J/mol×K	750.82	Joback Method
cpg	716.47	J/mol×K	783.07	Joback Method
cpg	731.47	J/mol×K	815.31	Joback Method
cpg	745.59	J/mol×K	847.56	Joback Method
cpg	758.88	J/mol×K	879.80	Joback Method

Sources

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=U308440&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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