

2-(Ethyl(m-tolyl)amino)ethyl (E)-2-methylbut-2-enoate

Inchi:	InChI=1S/C16H23NO2/c1-5-14(4)16(18)19-11-10-17(6-2)15-9-7-8-13(3)12-15/h5,7-9,12H
InchiKey:	INZDUNVAFSFLNG-LHHJGKSTSA-N
Formula:	C16H23NO2
SMILES:	CC=C(C)C(=O)OCCN(CC)c1cccc(C)c1
Mol. weight [g/mol]:	261.36

Physical Properties

Property code	Value	Unit	Source
gf	135.15	kJ/mol	Joback Method
hf	-218.35	kJ/mol	Joback Method
hfus	35.55	kJ/mol	Joback Method
hvap	65.39	kJ/mol	Joback Method
log10ws	-3.50		Crippen Method
logp	3.331		Crippen Method
mcvol	225.660	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinsol	1990.00		NIST Webbook
tb	689.91	K	Joback Method
tc	893.68	K	Joback Method
tf	394.61	K	Joback Method
vc	0.847	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	616.95	J/mol×K	689.91	Joback Method
cpg	633.86	J/mol×K	723.87	Joback Method
cpg	649.76	J/mol×K	757.83	Joback Method
cpg	664.69	J/mol×K	791.79	Joback Method
cpg	678.70	J/mol×K	825.76	Joback Method
cpg	691.84	J/mol×K	859.72	Joback Method
cpg	704.16	J/mol×K	893.68	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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=U373723&Units=SI

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
h vap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m cvol:	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

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