But-2-enamide, N-ethyl-N-(3-methylphenyl)-3-methyl-

Inchi: InChI=1S/C14H19NO/c1-5-15(14(16)9-11(2)3)13-8-6-7-12(4)10-13/h6-10H,5H2,1-4H3

InchiKey: OYOIGFDBZVQVAG-UHFFFAOYSA-N

Formula: C14H19NO

SMILES: CCN(C(=O)C=C(C)C)c1cccc(C)c1

Mol. weight [g/mol]: 217.31

Physical Properties

Property code	Value	Unit	Source
gf	223.31	kJ/mol	Joback Method
hf	-44.85	kJ/mol	Joback Method
hfus	29.18	kJ/mol	Joback Method
hvap	58.52	kJ/mol	Joback Method
log10ws	-3.58		Crippen Method
logp	3.314		Crippen Method
mcvol	191.610	ml/mol	McGowan Method
pc	2208.29	kPa	Joback Method
rinpol	1612.00		NIST Webbook
rinpol	1612.00		NIST Webbook
tb	621.73	K	Joback Method
tc	833.54	K	Joback Method
tf	349.84	K	Joback Method
vc	0.717	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	483.82	J/mol×K	621.73	Joback Method
cpg	500.42	J/mol×K	657.03	Joback Method
cpg	515.96	J/mol×K	692.33	Joback Method
cpg	530.51	J/mol×K	727.64	Joback Method
cpg	544.13	J/mol×K	762.94	Joback Method
cpg	556.89	J/mol×K	798.24	Joback Method
cpg	568.84	J/mol×K	833.54	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=U308236&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
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