Propanamide, 2,2-dimethyl-N-(3-methylphenyl)-

Other names: 2,2-Dimethyl-N-(3-methylphenyl)propanamide
Propanamide, N-(3-methylphenyl)-2,2-dimethyl-
Inchi: InChI=1S/C12H17NO/c1-9-6-5-7-10(8-9)13-11(14)12(2,3)4/h5-8H,1-4H3,(H,13,14)
InchiKey: OIJOHXNKDKMBCV-UHFFFAOYSA-N
Formula: C12H17NO
SMILES: Cc1cccc(NC(=O)C(C)(C)C)c1
Mol. weight [g/mol]: 191.27
CAS: 32597-29-8

Physical Properties

Property code	Value	Unit	Source
gf	116.25	kJ/mol	Joback Method
hf	-133.81	kJ/mol	Joback Method
hfus	19.77	kJ/mol	Joback Method
hvap	57.13	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.980		Crippen Method
mcvol	167.730	ml/mol	McGowan Method
pc	2605.74	kPa	Joback Method
rinpol	1524.00		NIST Webbook
tb	606.43	K	Joback Method
tc	827.99	K	Joback Method
tf	368.95	K	Joback Method
vc	0.629	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	422.85	J/mol×K	606.43	Joback Method
cpg	438.62	J/mol×K	643.36	Joback Method
cpg	453.30	J/mol×K	680.28	Joback Method
cpg	466.95	J/mol×K	717.21	Joback Method
cpg	479.65	J/mol×K	754.13	Joback Method
cpg	491.44	J/mol×K	791.06	Joback Method

cpg	502.40	J/mol×K	827.99	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C32597298&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

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