2-Butenamide, N-(4-methoxyphenyl)-3-methyl-

Inchi: InChI=1S/C12H15NO2/c1-9(2)8-12(14)13-10-4-6-11(15-3)7-5-10/h4-8H,1-3H3,(H,13,14)
InchiKey: GHNFZPUZIVOQFO-UHFFFAOYSA-N
Formula: C12H15NO2
SMILES: COc1ccc(NC(=O)C=C(C)C)cc1
Mol. weight [g/mol]: 205.25

Physical Properties

Property code	Value	Unit	Source
gf	80.08	kJ/mol	Joback Method
hf	-149.85	kJ/mol	Joback Method
hfus	27.27	kJ/mol	Joback Method
hvap	60.87	kJ/mol	Joback Method
log10ws	-2.90		Crippen Method
logp	2.600		Crippen Method
mcvol	169.300	ml/mol	McGowan Method
pc	2662.52	kPa	Joback Method
rinpol	1897.00		NIST Webbook
tb	636.12	K	Joback Method
tc	855.05	K	Joback Method
tf	369.72	K	Joback Method
vc	0.639	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.78	J/mol×K	636.12	Joback Method
cpg	438.08	J/mol×K	672.61	Joback Method
cpg	451.49	J/mol×K	709.10	Joback Method
cpg	464.02	J/mol×K	745.58	Joback Method
cpg	475.72	J/mol×K	782.07	Joback Method
cpg	486.64	J/mol×K	818.56	Joback Method
cpg	496.79	J/mol×K	855.05	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U307270&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

Latest version available from:
https://www.chemeo.com/cid/31-618-1/2-Butenamide-N-4-methoxyphenyl-3-methyl.pdf
Generated by Cheméo on 2024-10-12 08:51:16.155747964 +0000 UTC m=+3303938.792717213.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.