«alpha»-Methyl-«alpha»-phenylsuccinimide

Other names:	2,5-Pyrrolidinedione, 3-methyl-3-phenyl-
	Normethsuximide
	Desmethylmethsuximide
	Mesuximide, M(nor-)
	N-Demethylmethsuximide
	2-Methyl-2-phenylsuccinimide
	3-Methyl-3-phenyl-2,5-pyrrolidinedione
Inchi:	InChI=1S/C11H11NO2/c1-11(7-9(13)12-10(11)14)8-5-3-2-4-6-8/h2-6H,7H2,1H3,(H,12,13
InchiKey:	UDESUGJZUFALAM-UHFFFAOYSA-N
Formula:	C11H11NO2
SMILES:	CC1(c2ccccc2)CC(=O)NC1=O
Mol. weight [g/mol]:	189.21
CAS:	1497-17-2

Physical Properties

Property code	Value	Unit	Source
gf	27.74	kJ/mol	Joback Method
hf	-195.71	kJ/mol	Joback Method
hfus	14.53	kJ/mol	Joback Method
hvap	56.71	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	0.991		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	3796.32	kPa	Joback Method
rinpol	1649.00		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1652.00		NIST Webbook
tb	677.47	K	Joback Method
tc	956.20	K	Joback Method
tf	516.42	K	Joback Method
vc	0.533	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	385.66	J/mol×K	677.47	Joback Method
cpg	402.77	J/mol×K	723.93	Joback Method
cpg	418.87	J/mol×K	770.38	Joback Method
cpg	434.12	J/mol×K	816.84	Joback Method
cpg	448.63	J/mol×K	863.29	Joback Method
cpg	462.56	J/mol×K	909.75	Joback Method
cpg	476.02	J/mol×K	956.20	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1497172&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
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

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