Propanediamide, 2-ethyl-2-phenyl-

Other names:	Malonamide, 2-ethyl-2-phenyl-
	Ethylphenylmalondiamide
	Phenylethylmalonamide
	Phenylethylmalondiamide
	2-Ethyl-2-phenylmalondiamide
	2-Ethyl-2-phenylmalonamide
	2-Ethyl-2-phenylmalonic diamide
	PEMA
	PEMA (amide)
	80866-90-6 (hydrate)
	Primidone, M(diamide)
	2-ethyl-2-phenylmalonamide monohydrate
Inchi:	InChI=1S/C11H14N2O2/c1-2-11(9(12)14,10(13)15)8-6-4-3-5-7-8/h3-7H,2H2,1H3,(H2,12
InchiKey:	JFZHPFOXAAIUMB-UHFFFAOYSA-N
Formula:	C11H14N2O2
SMILES:	CCC(C(N)=O)(C(N)=O)c1ccccc1
Mol. weight [g/mol]:	206.24
CAS:	7206-76-0

Physical Properties

Property code	Value	Unit	Source
gf	32.05	kJ/mol	Joback Method
hf	-200.17	kJ/mol	Joback Method
hfus	24.46	kJ/mol	Joback Method
hvap	75.83	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	0.305		Crippen Method
mcvol	165.190	ml/mol	McGowan Method
pc	3526.27	kPa	Joback Method
rinpol	1916.00		NIST Webbook
rinpol	1916.00		NIST Webbook
rinpol	1935.00		NIST Webbook
tb	727.33	K	Joback Method
tc	972.77	K	Joback Method
tf	508.95	K	Joback Method
vc	0.603	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.02	J/mol×K	727.33	Joback Method
cpg	468.20	J/mol×K	768.24	Joback Method
cpg	479.30	J/mol×K	809.14	Joback Method
cpg	489.44	J/mol×K	850.05	Joback Method
cpg	498.70	J/mol×K	890.96	Joback Method
cpg	507.16	J/mol×K	931.86	Joback Method
cpg	514.93	J/mol×K	972.77	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=C7206760&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