2,4-Azetidinedione, 3-ethyl-3-phenyl-

Other names: Malonimide, 2-ethyl-2-phenyl-
3-Ethyl-3-phenylazetidin-2,4-dione
Inchi: InChI=1S/C11H11NO2/c1-2-11(9(13)12-10(11)14)8-6-4-3-5-7-8/h3-7H,2H2,1H3,(H,12,13
InchiKey: DBNSSSWQTICKIC-UHFFFAOYSA-N
Formula: C11H11NO2
SMILES: CCC1(c2ccccc2)C(=O)NC1=O
Mol. weight [g/mol]: 189.21
CAS: 42282-82-6

Physical Properties

Property code	Value	Unit	Source
gf	39.84	kJ/mol	Joback Method
hf	-189.55	kJ/mol	Joback Method
hfus	16.63	kJ/mol	Joback Method
hvap	56.54	kJ/mol	Joback Method
ie	8.90	eV	NIST Webbook
log10ws	-1.84		Crippen Method
logp	0.991		Crippen Method
mcvol	144.350	ml/mol	McGowan Method
pc	3682.02	kPa	Joback Method
tb	673.20	K	Joback Method
tc	942.49	K	Joback Method
tf	519.94	K	Joback Method
vc	0.541	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	383.71	J/mol×K	673.20	Joback Method
cpg	399.83	J/mol×K	718.08	Joback Method
cpg	415.08	J/mol×K	762.96	Joback Method
cpg	429.59	J/mol×K	807.84	Joback Method
cpg	443.50	J/mol×K	852.73	Joback Method
cpg	456.94	J/mol×K	897.61	Joback Method

cpg	470.07	J/mol×K	942.49	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=C42282826&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
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume