2,4-Azetidinedione, 3,3-diethyl-

Other names:	Malonimide, 2,2-diethyl-
	3,3-Diethylazetidin-2,4-dione
Inchi:	InChI=1S/C7H11NO2/c1-3-7(4-2)5(9)8-6(7)10/h3-4H2,1-2H3,(H,8,9,10)
InchiKey:	OQYOLDLENQHHFM-UHFFFAOYSA-N
Formula:	C7H11NO2
SMILES:	CCC1(CC)C(=O)NC1=O
Mol. weight [g/mol]:	141.17
CAS:	42282-85-9

Physical Properties

Property code	Value	Unit	Source
gf	-106.25	kJ/mol	Joback Method
hf	-343.52	kJ/mol	Joback Method
hfus	12.23	kJ/mol	Joback Method
hvap	45.36	kJ/mol	Joback Method
ie	9.57	eV	NIST Webbook
log10ws	-1.15		Crippen Method
logp	0.449		Crippen Method
mcvol	111.750	ml/mol	McGowan Method
pc	3930.78	kPa	Joback Method
tb	555.00	K	Joback Method
tc	793.42	K	Joback Method
tf	448.44	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	270.64	J/mol×K	555.00	Joback Method
cpg	284.12	J/mol×K	594.74	Joback Method
cpg	296.99	J/mol×K	634.47	Joback Method
cpg	309.33	J/mol×K	674.21	Joback Method
cpg	321.19	J/mol×K	713.95	Joback Method
cpg	332.65	J/mol×K	753.69	Joback Method

cpg	343.77	J/mol×K	793.42	Joback Method

Sources

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=C42282859&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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