Diethyl 2-(2-cyanoethyl)-malonate

Other names:	Diethyl (2-cyanoethyl)malonate
	Propanedioic acid, (2-cyanoethyl)-, diethyl ester
	Diethyl 2-cyanomalonate
Inchi:	InChI=1S/C10H15NO4/c1-3-14-9(12)8(6-5-7-11)10(13)15-4-2/h8H,3-6H2,1-2H3
InchiKey:	YJJLOESDBPRZIP-UHFFFAOYSA-N
Formula:	C10H15NO4
SMILES:	CCOC(=O)C(CCC#N)C(=O)OCC
Mol. weight [g/mol]:	213.23
CAS:	17216-62-5

Physical Properties

Property code	Value	Unit	Source
gf	-303.78	kJ/mol	Joback Method
hf	-579.73	kJ/mol	Joback Method
hfus	25.21	kJ/mol	Joback Method
hvap	66.26	kJ/mol	Joback Method
log10ws	-1.36		Crippen Method
logp	1.033		Crippen Method
mcvol	168.020	ml/mol	McGowan Method
pc	2261.11	kPa	Joback Method
tb	682.42	K	Joback Method
tc	879.91	K	Joback Method
tf	396.77	K	Joback Method
vc	0.663	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	443.83	J/mol×K	682.42	Joback Method
cpg	455.26	J/mol×K	715.33	Joback Method
cpg	466.06	J/mol×K	748.25	Joback Method
cpg	476.23	J/mol×K	781.16	Joback Method
cpg	485.76	J/mol×K	814.08	Joback Method
cpg	494.65	J/mol×K	846.99	Joback Method

cpg	502.88	J/mol×K	879.91	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	388.70	K	0.30	NIST Webbook

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=C17216625&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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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