

Diethylmalonic acid, butyl 2-nitrophenyl ester

Inchi:	InChI=1S/C17H23NO6/c1-4-7-12-23-15(19)17(5-2,6-3)16(20)24-14-11-9-8-10-13(14)18(
InchiKey:	UCZSXQWHWRZMEK-UHFFFAOYSA-N
Formula:	C17H23NO6
SMILES:	CCCCOC(=O)C(CC)(CC)C(=O)Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	337.37

Physical Properties

Property code	Value	Unit	Source
gf	-234.41	kJ/mol	Joback Method
hf	-678.26	kJ/mol	Joback Method
hfus	42.96	kJ/mol	Joback Method
hvap	89.98	kJ/mol	Joback Method
log10ws	-4.82		Crippen Method
logp	3.650		Crippen Method
mvol	258.930	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2264.00		NIST Webbook
rinpol	2264.00		NIST Webbook
tb	921.21	K	Joback Method
tc	1149.56	K	Joback Method
tf	610.64	K	Joback Method
vc	0.999	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.12	J/molxK	921.21	Joback Method
cpg	825.55	J/molxK	959.27	Joback Method
cpg	836.80	J/molxK	997.33	Joback Method
cpg	846.92	J/molxK	1035.39	Joback Method
cpg	855.96	J/molxK	1073.45	Joback Method
cpg	863.98	J/molxK	1111.51	Joback Method
cpg	871.02	J/molxK	1149.56	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U369858&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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