

Diethylmalonic acid, butyl 4-nitrophenyl ester

Inchi:

InChI=1S/C17H23NO6/c1-4-7-12-23-15(19)17(5-2,6-3)16(20)24-14-10-8-13(9-11-14)18(

InchiKey:

MFSWWEUNLNXTPX-UHFFFAOYSA-N

Formula:

C17H23NO6

SMILES:

CCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc([N+](=O)[O-])cc1

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
mcvol	258.930	ml/mol	McGowan Method
pc	1720.31	kPa	Joback Method
rinpol	2268.00		NIST Webbook
tb	921.21	K	Joback Method
tc	1149.56	K	Joback Method
tf	610.64	K	Joback Method
vc	0.999	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	813.12	J/mol×K	921.21	Joback Method
cpg	825.55	J/mol×K	959.27	Joback Method
cpg	836.80	J/mol×K	997.33	Joback Method
cpg	846.92	J/mol×K	1035.39	Joback Method
cpg	855.96	J/mol×K	1073.45	Joback Method
cpg	863.98	J/mol×K	1111.51	Joback Method
cpg	871.02	J/mol×K	1149.56	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=U370163&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
hvac:	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

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