

Glutaric acid, di(2-nitrophenyl) ester

Inchi:	InChI=1S/C17H14N2O8/c20-16(26-14-8-3-1-6-12(14)18(22)23)10-5-11-17(21)27-15-9-4
InchiKey:	JYMGOHDYCGYCDU-UHFFFAOYSA-N
Formula:	C17H14N2O8
SMILES:	O=C(CCCC(=O)Oc1ccccc1[N+](=O)[O-])Oc1ccccc1[N+](=O)[O-]
Mol. weight [g/mol]:	374.30

Physical Properties

Property code	Value	Unit	Source
gf	-98.92	kJ/mol	Joback Method
hf	-455.21	kJ/mol	Joback Method
hfus	55.39	kJ/mol	Joback Method
hvap	110.81	kJ/mol	Joback Method
log10ws	-5.47		Crippen Method
logp	3.184		Crippen Method
mcvol	252.590	ml/mol	McGowan Method
pc	2263.26	kPa	Joback Method
rinpola	3166.00		NIST Webbook
tb	1107.94	K	Joback Method
tc	1375.35	K	Joback Method
tf	790.77	K	Joback Method
vc	0.984	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	779.53	J/molxK	1107.94	Joback Method
cpg	784.66	J/molxK	1152.51	Joback Method
cpg	788.33	J/molxK	1197.08	Joback Method
cpg	790.60	J/molxK	1241.64	Joback Method
cpg	791.53	J/molxK	1286.21	Joback Method
cpg	791.17	J/molxK	1330.78	Joback Method
cpg	789.57	J/molxK	1375.35	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=U358761&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
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mccvol:	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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