

Glutaric acid, 4-methyl-3-nitrobenzyl pentyl ester

Inchi:	InChI=1S/C18H25NO6/c1-3-4-5-11-24-17(20)7-6-8-18(21)25-13-15-10-9-14(2)16(12-15)
InchiKey:	SPDDQRQQSPKFTA-UHFFFAOYSA-N
Formula:	C18H25NO6
SMILES:	CCCCCOC(=O)CCCC(=O)OCc1ccc(C)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	351.39

Physical Properties

Property code	Value	Unit	Source
gf	-238.46	kJ/mol	Joback Method
hf	-701.62	kJ/mol	Joback Method
hfus	52.57	kJ/mol	Joback Method
hvap	94.17	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	3.850		Crippen Method
mcvol	273.020	ml/mol	McGowan Method
pc	1548.78	kPa	Joback Method
rinpol	2671.00		NIST Webbook
rinpol	2671.00		NIST Webbook
tb	952.30	K	Joback Method
tc	1175.63	K	Joback Method
tf	632.01	K	Joback Method
vc	1.065	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	869.16	J/mol×K	952.30	Joback Method
cpg	881.41	J/mol×K	989.52	Joback Method
cpg	892.39	J/mol×K	1026.74	Joback Method
cpg	902.11	J/mol×K	1063.97	Joback Method
cpg	910.59	J/mol×K	1101.19	Joback Method
cpg	917.87	J/mol×K	1138.41	Joback Method
cpg	923.95	J/mol×K	1175.63	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=U376781&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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