

Glutaric acid, heptyl 3-nitrobenzyl ester

Inchi:	InChI=1S/C19H27NO6/c1-2-3-4-5-6-13-25-18(21)11-8-12-19(22)26-15-16-9-7-10-17(14-
InchiKey:	XUHDYUUKXBCACF-UHFFFAOYSA-N
Formula:	C19H27NO6
SMILES:	CCCCCCCOC(=O)CCCC(=O)OCc1cccc([N+](=O)[O-])c1
Mol. weight [g/mol]:	365.42

Physical Properties

Property code	Value	Unit	Source
gf	-220.41	kJ/mol	Joback Method
hf	-710.79	kJ/mol	Joback Method
hfus	55.55	kJ/mol	Joback Method
hvap	95.73	kJ/mol	Joback Method
log10ws	-5.75		Crippen Method
logp	4.322		Crippen Method
mvol	287.110	ml/mol	McGowan Method
pc	1454.57	kPa	Joback Method
rinpol	2910.00		NIST Webbook
rinpol	2910.00		NIST Webbook
tb	970.20	K	Joback Method
tc	1193.92	K	Joback Method
tf	630.76	K	Joback Method
vc	1.121	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	929.17	J/mol×K	970.20	Joback Method
cpg	941.66	J/mol×K	1007.49	Joback Method
cpg	952.85	J/mol×K	1044.77	Joback Method
cpg	962.77	J/mol×K	1082.06	Joback Method
cpg	971.45	J/mol×K	1119.34	Joback Method
cpg	978.94	J/mol×K	1156.63	Joback Method
cpg	985.26	J/mol×K	1193.92	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U377465&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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