

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

Inchi:	InChI=1S/C25H39NO6/c1-3-4-5-6-7-8-9-10-11-12-18-31-24(27)14-13-15-25(28)32-20-22
InchiKey:	QDLIOWIGKDYQGV-UHFFFAOYSA-N
Formula:	C25H39NO6
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(C)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	449.58

Physical Properties

Property code	Value	Unit	Source
gf	-179.52	kJ/mol	Joback Method
hf	-846.10	kJ/mol	Joback Method
hfus	70.70	kJ/mol	Joback Method
hvap	109.75	kJ/mol	Joback Method
log10ws	-8.32		Crippen Method
logp	6.581		Crippen Method
mcvol	371.650	ml/mol	McGowan Method
pc	968.68	kPa	Joback Method
rinpola	3397.00		NIST Webbook
tb	1112.46	K	Joback Method
tc	1366.14	K	Joback Method
tf	710.90	K	Joback Method
vc	1.458	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1289.76	J/molxK	1112.46	Joback Method
cpg	1302.71	J/molxK	1154.74	Joback Method
cpg	1313.81	J/molxK	1197.02	Joback Method
cpg	1323.12	J/molxK	1239.30	Joback Method
cpg	1330.72	J/molxK	1281.58	Joback Method
cpg	1336.68	J/molxK	1323.86	Joback Method
cpg	1341.06	J/molxK	1366.14	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376789&Units=SI
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

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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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