

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

Inchi:	InChI=1S/C26H41NO6/c1-3-4-5-6-7-8-9-10-11-12-13-19-32-25(28)15-14-16-26(29)33-21
InchiKey:	BVTPZWWYVSBMRM-UHFFFAOYSA-N
Formula:	C26H41NO6
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(C)c([N+](=O)[O-])c1
Mol. weight [g/mol]:	463.61

Physical Properties

Property code	Value	Unit	Source
gf	-171.10	kJ/mol	Joback Method
hf	-866.74	kJ/mol	Joback Method
hfus	73.29	kJ/mol	Joback Method
hvap	111.97	kJ/mol	Joback Method
log10ws	-8.74		Crippen Method
logp	6.971		Crippen Method
mcvol	385.740	ml/mol	McGowan Method
pc	913.29	kPa	Joback Method
rinpol	3505.00		NIST Webbook
rinpol	3505.00		NIST Webbook
tb	1135.34	K	Joback Method
tc	1398.10	K	Joback Method
tf	722.17	K	Joback Method
vc	1.514	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1351.25	J/mol×K	1135.34	Joback Method
cpg	1364.32	J/mol×K	1179.13	Joback Method
cpg	1375.40	J/mol×K	1222.93	Joback Method
cpg	1384.57	J/mol×K	1266.72	Joback Method
cpg	1391.92	J/mol×K	1310.51	Joback Method
cpg	1397.52	J/mol×K	1354.31	Joback Method
cpg	1401.47	J/mol×K	1398.10	Joback Method

Sources

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=U376790&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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