

Glutaric acid, monoamide, N-(4-methylbenzyl)-, tetradecyl ester

Inchi: InChI=1S/C27H45NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-22-31-27(30)17-15-16-26(29)28
InchiKey: RWEVFGQFGDLGES-UHFFFAOYSA-N
Formula: C27H45NO3
SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)NCc1ccc(C)cc1
Mol. weight [g/mol]: 431.65

Physical Properties

Property code	Value	Unit	Source
gf	5.79	kJ/mol	Joback Method
hf	-679.46	kJ/mol	Joback Method
hfus	68.82	kJ/mol	Joback Method
hvap	100.97	kJ/mol	Joback Method
log10ws	-8.61		Crippen Method
logp	7.026		Crippen Method
mcvol	386.520	ml/mol	McGowan Method
pc	879.48	kPa	Joback Method
rinpol	3481.00		NIST Webbook
tb	1029.15	K	Joback Method
tc	1263.95	K	Joback Method
tf	607.74	K	Joback Method
vc	1.504	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1338.65	J/mol×K	1029.15	Joback Method
cpg	1356.67	J/mol×K	1068.28	Joback Method
cpg	1373.12	J/mol×K	1107.42	Joback Method
cpg	1388.09	J/mol×K	1146.55	Joback Method
cpg	1401.66	J/mol×K	1185.68	Joback Method
cpg	1413.93	J/mol×K	1224.81	Joback Method
cpg	1424.98	J/mol×K	1263.95	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=U360020&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
mcvol:	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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