

Glutaric acid, monoamide, N,N-di(4-methylphenyl)-, nonyl ester

Inchi:	InChI=1S/C28H39NO3/c1-4-5-6-7-8-9-10-22-32-28(31)13-11-12-27(30)29(25-18-14-23(2
InchiKey:	ANFLCNXUCGADNH-UHFFFAOYSA-N
Formula:	C28H39NO3
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)N(c1ccc(C)cc1)c1ccc(C)cc1
Mol. weight [g/mol]:	437.61

Physical Properties

Property code	Value	Unit	Source
gf	138.38	kJ/mol	Joback Method
hf	-460.98	kJ/mol	Joback Method
hfus	62.99	kJ/mol	Joback Method
hvap	101.74	kJ/mol	Joback Method
log10ws	-8.21		Crippen Method
logp	7.432		Crippen Method
mvol	376.850	ml/mol	McGowan Method
pc	997.02	kPa	Joback Method
rinpol	3302.00		NIST Webbook
rinpol	3302.00		NIST Webbook
tb	1045.96	K	Joback Method
tc	1280.55	K	Joback Method
tf	637.76	K	Joback Method
vc	1.435	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1275.87	J/mol×K	1045.96	Joback Method
cpg	1291.73	J/mol×K	1085.06	Joback Method
cpg	1306.20	J/mol×K	1124.16	Joback Method
cpg	1319.38	J/mol×K	1163.25	Joback Method
cpg	1331.37	J/mol×K	1202.35	Joback Method
cpg	1342.28	J/mol×K	1241.45	Joback Method
cpg	1352.21	J/mol×K	1280.55	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=U360238&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
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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