

Glutaric acid, monoamide, N-(2-phenylpropyl)-, tetradecyl ester

Inchi: InChI=1S/C28H47NO3/c1-3-4-5-6-7-8-9-10-11-12-13-17-23-32-28(31)22-18-21-27(30)29

InchiKey: MCUZXYWGBZSWBK-UHFFFAOYSA-N

Formula: C28H47NO3

SMILES: CCCCCCCCCCCCCCOC(=O)CCCC(=O)NCC(C)c1ccccc1

Mol. weight [g/mol]: 445.68

Physical Properties

Property code	Value	Unit	Source
gf	21.40	kJ/mol	Joback Method
hf	-693.91	kJ/mol	Joback Method
hfus	68.28	kJ/mol	Joback Method
hvap	102.15	kJ/mol	Joback Method
log10ws	-8.44		Crippen Method
logp	7.321		Crippen Method
mcvol	400.610	ml/mol	McGowan Method
pc	842.60	kPa	Joback Method
rinpol	3466.00		NIST Webbook
rinpol	3466.00		NIST Webbook
tb	1046.61	K	Joback Method
tc	1287.21	K	Joback Method
tf	591.49	K	Joback Method
vc	1.554	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1402.96	J/mol×K	1046.61	Joback Method
cpg	1421.42	J/mol×K	1086.71	Joback Method
cpg	1438.25	J/mol×K	1126.81	Joback Method
cpg	1453.56	J/mol×K	1166.91	Joback Method
cpg	1467.46	J/mol×K	1207.01	Joback Method
cpg	1480.07	J/mol×K	1247.11	Joback Method
cpg	1491.49	J/mol×K	1287.21	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360831&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
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
rlnpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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