

Glutaric acid, monoamide, N-(1-phenylethyl)-, heptadecyl ester

Inchi: InChI=1S/C30H51NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-20-26-34-30(33)25-21-24

InchiKey: DVKCWJGETRAZTC-UHFFFAOYSA-N

Formula: C30H51NO3

SMILES: CCCCCCCCCCCCCCCCCOC(=O)CCCC(=O)NC(C)c1ccccc1

Mol. weight [g/mol]: 473.73

Physical Properties

Property code	Value	Unit	Source
gf	38.24	kJ/mol	Joback Method
hf	-735.19	kJ/mol	Joback Method
hfus	73.46	kJ/mol	Joback Method
hvap	106.60	kJ/mol	Joback Method
log10ws	-9.77		Crippen Method
logp	8.449		Crippen Method
mcvol	428.790	ml/mol	McGowan Method
pc	755.99	kPa	Joback Method
rinpol	2897.00		NIST Webbook
tb	1092.37	K	Joback Method
tc	1353.54	K	Joback Method
tf	614.03	K	Joback Method
vc	1.667	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1530.82	J/mol×K	1092.37	Joback Method
cpg	1550.35	J/mol×K	1135.90	Joback Method
cpg	1568.02	J/mol×K	1179.43	Joback Method
cpg	1583.98	J/mol×K	1222.96	Joback Method
cpg	1598.38	J/mol×K	1266.49	Joback Method
cpg	1611.37	J/mol×K	1310.01	Joback Method
cpg	1623.11	J/mol×K	1353.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360165&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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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