

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

Inchi: InChI=1S/C23H37NO3/c1-3-4-5-6-7-8-9-13-19-27-23(26)18-14-17-22(25)24-20(2)21-15-
InchiKey: FKUKQWNTLCRMCR-UHFFFAOYSA-N
Formula: C23H37NO3
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)NC(C)c1ccccc1
Mol. weight [g/mol]: 375.54

Physical Properties

Property code	Value	Unit	Source
gf	-20.70	kJ/mol	Joback Method
hf	-590.71	kJ/mol	Joback Method
hfus	55.33	kJ/mol	Joback Method
hvap	91.02	kJ/mol	Joback Method
log10ws	-6.84		Crippen Method
logp	5.718		Crippen Method
mcvol	330.160	ml/mol	McGowan Method
pc	1137.50	kPa	Joback Method
rinpol	2920.00		NIST Webbook
rinpol	2920.00		NIST Webbook
tb	932.21	K	Joback Method
tc	1142.86	K	Joback Method
tf	535.14	K	Joback Method
vc	1.274	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1090.30	J/mol×K	932.21	Joback Method
cpg	1106.97	J/mol×K	967.32	Joback Method
cpg	1122.39	J/mol×K	1002.43	Joback Method
cpg	1136.61	J/mol×K	1037.53	Joback Method
cpg	1149.69	J/mol×K	1072.64	Joback Method
cpg	1161.70	J/mol×K	1107.75	Joback Method
cpg	1172.69	J/mol×K	1142.86	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360160&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I
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
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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