

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

Inchi: InChI=1S/C24H39NO3/c1-3-4-5-6-7-8-9-13-19-28-24(27)18-14-17-23(26)25-20-21(2)22-
InchiKey: CWYANFVJUDVLRC-UHFFFAOYSA-N
Formula: C24H39NO3
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)NCC(C)c1ccccc1
Mol. weight [g/mol]: 389.57

Physical Properties

Property code	Value	Unit	Source
gf	-12.28	kJ/mol	Joback Method
hf	-611.35	kJ/mol	Joback Method
hfus	57.92	kJ/mol	Joback Method
hvap	93.24	kJ/mol	Joback Method
log10ws	-6.76		Crippen Method
logp	5.760		Crippen Method
mcvol	344.250	ml/mol	McGowan Method
pc	1067.27	kPa	Joback Method
rinpol	3044.00		NIST Webbook
rinpol	3044.00		NIST Webbook
tb	955.09	K	Joback Method
tc	1169.60	K	Joback Method
tf	546.41	K	Joback Method
vc	1.331	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1151.88	J/mol×K	955.09	Joback Method
cpg	1168.83	J/mol×K	990.84	Joback Method
cpg	1184.46	J/mol×K	1026.59	Joback Method
cpg	1198.86	J/mol×K	1062.35	Joback Method
cpg	1212.08	J/mol×K	1098.10	Joback Method
cpg	1224.18	J/mol×K	1133.85	Joback Method
cpg	1235.23	J/mol×K	1169.60	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360828&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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