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

Inchi: InChI=1S/C26H43NO3/c1-3-4-5-6-7-8-9-10-11-15-21-30-26(29)20-16-19-25(28)27-22-23

InchiKey: OODZBKQOTSBHAV-UHFFFAOYSA-N

Formula: C26H43NO3

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

Mol. weight [g/mol]: 417.62

Physical Properties

Property code	Value	Unit	Source
gf	4.56	kJ/mol	Joback Method
hf	-652.63	kJ/mol	Joback Method
hfus	63.10	kJ/mol	Joback Method
hvap	97.70	kJ/mol	Joback Method
log10ws	-7.60		Crippen Method
logp	6.541		Crippen Method
mcvol	372.430	ml/mol	McGowan Method
pc	945.00	kPa	Joback Method
rinpol	3248.00		NIST Webbook
tb	1000.85	K	Joback Method
tc	1226.13	K	Joback Method
tf	568.95	K	Joback Method
vc	1.442	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1276.55	J/mol×K	1000.85	Joback Method
cpg	1294.16	J/mol×K	1038.40	Joback Method
cpg	1310.32	J/mol×K	1075.94	Joback Method
cpg	1325.12	J/mol×K	1113.49	Joback Method
cpg	1338.65	J/mol×K	1151.04	Joback Method
cpg	1350.97	J/mol×K	1188.58	Joback Method
cpg	1362.18	J/mol×K	1226.13	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=U360830&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume