Glutaric acid, monoamide, N-dodecyl-, pentyl ester

Inchi: InChI=1S/C22H43NO3/c1-3-5-7-8-9-10-11-12-13-14-19-23-21(24)17-16-18-22(25)26-20-
InchiKey: RFBOEUXUCFUUGJ-UHFFFAOYSA-N
Formula: C22H43NO3
SMILES: CCCCCCCCCCCCNC(=O)CCCC(=O)OCCCCC
Mol. weight [g/mol]: 369.58

Physical Properties

Property code	Value	Unit	Source
gf	-139.09	kJ/mol	Joback Method
hf	-801.32	kJ/mol	Joback Method
hfus	62.22	kJ/mol	Joback Method
hvap	86.90	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.927		Crippen Method
mcvol	339.830	ml/mol	McGowan Method
pc	971.70	kPa	Joback Method
rinpol	3208.00		NIST Webbook
rinpol	3208.00		NIST Webbook
tb	883.09	K	Joback Method
tc	1081.24	K	Joback Method
tf	512.45	K	Joback Method
vc	1.333	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1125.66	J/mol×K	883.09	Joback Method
cpg	1144.72	J/mol×K	916.11	Joback Method
cpg	1162.56	J/mol×K	949.14	Joback Method
cpg	1179.23	J/mol×K	982.16	Joback Method
cpg	1194.77	J/mol×K	1015.19	Joback Method
cpg	1209.21	J/mol×K	1048.21	Joback Method
cpg	1222.61	J/mol×K	1081.24	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360869&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