Glutaric acid, monoamide, N-(2-octyl)-, tridecyl ester

Inchi: InChI=1S/C26H51NO3/c1-4-6-8-10-11-12-13-14-15-16-18-23-30-26(29)22-19-21-25(28)2
InchiKey: CKNMTUAGGPAZCO-UHFFFAOYSA-N
Formula: C26H51NO3
SMILES: CCCCCCCCCCCCCOC(=O)CCCC(=O)NC(C)CCCCCC
Mol. weight [g/mol]: 425.69

Physical Properties

Property code	Value	Unit	Source
gf	-107.85	kJ/mol	Joback Method
hf	-889.16	kJ/mol	Joback Method
hfus	69.06	kJ/mol	Joback Method
hvap	95.42	kJ/mol	Joback Method
log10ws	-8.64		Crippen Method
logp	7.486		Crippen Method
mcvol	396.190	ml/mol	McGowan Method
pc	778.51	kPa	Joback Method
rinpol	3446.00		NIST Webbook
rinpol	3446.00		NIST Webbook
tb	974.17	K	Joback Method
tc	1201.26	K	Joback Method
tf	542.53	K	Joback Method
vc	1.550	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1379.94	J/mol×K	974.17	Joback Method
cpg	1401.24	J/mol×K	1012.02	Joback Method
cpg	1420.89	J/mol×K	1049.87	Joback Method
cpg	1438.95	J/mol×K	1087.72	Joback Method
cpg	1455.51	J/mol×K	1125.57	Joback Method
cpg	1470.63	J/mol×K	1163.42	Joback Method
cpg	1484.40	J/mol×K	1201.26	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360861&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

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