

Glutaric acid, dodec-9-ynyl octyl ester

Inchi: InChI=1S/C25H44O4/c1-3-5-7-9-11-12-13-14-16-18-23-29-25(27)21-19-20-24(26)28-22-
InchiKey: KMFIGQCPMADFIZ-UHFFFAOYSA-N
Formula: C25H44O4
SMILES: CCC#CCCCCCCCCOC(=O)CCCC(=O)OCCCCCCCCC
Mol. weight [g/mol]: 408.61

Physical Properties

Property code	Value	Unit	Source
gf	-105.42	kJ/mol	Joback Method
hf	-776.63	kJ/mol	Joback Method
hfus	69.20	kJ/mol	Joback Method
hvap	91.71	kJ/mol	Joback Method
log10ws	-7.81		Crippen Method
logp	6.748		Crippen Method
mcvol	369.390	ml/mol	McGowan Method
pc	882.62	kPa	Joback Method
rinpol	2954.00		NIST Webbook
rinpol	2954.00		NIST Webbook
tb	932.98	K	Joback Method
tc	1142.70	K	Joback Method
tf	621.93	K	Joback Method
vc	1.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1227.56	J/mol×K	932.98	Joback Method
cpg	1246.71	J/mol×K	967.93	Joback Method
cpg	1264.43	J/mol×K	1002.89	Joback Method
cpg	1280.75	J/mol×K	1037.84	Joback Method
cpg	1295.72	J/mol×K	1072.80	Joback Method
cpg	1309.36	J/mol×K	1107.75	Joback Method
cpg	1321.71	J/mol×K	1142.70	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359791&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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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