

Glutaric acid, dodecyl 2-methyloct-5-yn-4-yl ester

Inchi:	InChI=1S/C26H46O4/c1-5-7-9-10-11-12-13-14-15-16-21-29-25(27)19-17-20-26(28)30-24
InchiKey:	OAUFKDANARNWOV-UHFFFAOYSA-N
Formula:	C26H46O4
SMILES:	CCC#CC(CC(C)C)OC(=O)CCCC(=O)OCCCCCCCCCCCCC
Mol. weight [g/mol]:	422.64

Physical Properties

Property code	Value	Unit	Source
gf	-101.88	kJ/mol	Joback Method
hf	-807.83	kJ/mol	Joback Method
hfus	64.75	kJ/mol	Joback Method
hvap	93.16	kJ/mol	Joback Method
log10ws	-8.10		Crippen Method
logp	6.992		Crippen Method
mcvol	383.480	ml/mol	McGowan Method
pc	842.11	kPa	Joback Method
rinpola	3640.00		NIST Webbook
tb	954.98	K	Joback Method
tc	1169.90	K	Joback Method
tf	603.20	K	Joback Method
vc	1.490	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1291.58	J/mol×K	954.98	Joback Method
cpg	1310.96	J/mol×K	990.80	Joback Method
cpg	1328.79	J/mol×K	1026.62	Joback Method
cpg	1345.11	J/mol×K	1062.44	Joback Method
cpg	1359.96	J/mol×K	1098.26	Joback Method
cpg	1373.38	J/mol×K	1134.08	Joback Method
cpg	1385.42	J/mol×K	1169.90	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359609&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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
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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