

Glutaric acid, hex-2-en-1-yl tridec-2-yn-1-yl ester

Inchi:	InChI=1S/C24H40O4/c1-3-5-7-9-10-11-12-13-14-15-17-22-28-24(26)20-18-19-23(25)27-
InchiKey:	PXNQAOWRZJPETA-LZYBPNLTSA-N
Formula:	C24H40O4
SMILES:	CCCC=CCOC(=O)CCCC(=O)OCC#CCCCCCCCCCC
Mol. weight [g/mol]:	392.57

Physical Properties

Property code	Value	Unit	Source
gf	-33.62	kJ/mol	Joback Method
hf	-638.77	kJ/mol	Joback Method
hfus	66.81	kJ/mol	Joback Method
hvap	89.44	kJ/mol	Joback Method
log10ws	-7.24		Crippen Method
logp	6.134		Crippen Method
mcvol	351.000	ml/mol	McGowan Method
pc	965.67	kPa	Joback Method
rinpol	2760.00		NIST Webbook
rinpol	2760.00		NIST Webbook
tb	914.26	K	Joback Method
tc	1119.52	K	Joback Method
tf	605.58	K	Joback Method
vc	1.369	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1137.42	J/mol×K	914.26	Joback Method
cpg	1155.66	J/mol×K	948.47	Joback Method
cpg	1172.68	J/mol×K	982.68	Joback Method
cpg	1188.52	J/mol×K	1016.89	Joback Method
cpg	1203.23	J/mol×K	1051.10	Joback Method
cpg	1216.84	J/mol×K	1085.31	Joback Method
cpg	1229.39	J/mol×K	1119.52	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405341&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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