

Glutaric acid, 2,4-dimethylpent-3-yl undecyl ester

Inchi:	InChI=1S/C23H44O4/c1-6-7-8-9-10-11-12-13-14-18-26-21(24)16-15-17-22(25)27-23(19)
InchiKey:	KJFSBJAUPMHRKK-UHFFFAOYSA-N
Formula:	C23H44O4
SMILES:	CCCCCCCCCOC(=O)CCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	384.59

Physical Properties

Property code	Value	Unit	Source
gf	-332.38	kJ/mol	Joback Method
hf	-1023.49	kJ/mol	Joback Method
hfus	50.33	kJ/mol	Joback Method
hvap	83.94	kJ/mol	Joback Method
log10ws	-6.80		Crippen Method
logp	6.454		Crippen Method
mcvol	349.810	ml/mol	McGowan Method
pc	912.73	kPa	Joback Method
rinqol	2555.00		NIST Webbook
tb	876.90	K	Joback Method
tc	1073.65	K	Joback Method
tf	448.29	K	Joback Method
vc	1.353	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1155.84	J/molxK	876.90	Joback Method
cpg	1240.78	J/molxK	1040.85	Joback Method
cpg	1226.32	J/molxK	1008.06	Joback Method
cpg	1210.62	J/molxK	975.27	Joback Method
cpg	1193.66	J/molxK	942.48	Joback Method
cpg	1175.41	J/molxK	909.69	Joback Method
cpg	1254.03	J/molxK	1073.65	Joback Method
dvisc	0.0000262	Paxs	876.90	Joback Method
dvisc	0.0000367	Paxs	805.47	Joback Method

dvisc	0.0000548	Paxs	734.03	Joback Method
dvisc	0.0000894	Paxs	662.60	Joback Method
dvisc	0.0001639	Paxs	591.16	Joback Method
dvisc	0.0003551	Paxs	519.73	Joback Method
dvisc	0.0009847	Paxs	448.29	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359483&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

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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

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