

Succinic acid, 2,4-dimethylpent-3-yl tridecyl ester

Inchi:	InChI=1S/C24H46O4/c1-6-7-8-9-10-11-12-13-14-15-16-19-27-22(25)17-18-23(26)28-24(
InchiKey:	PTKRMGSCPPZYCL-UHFFFAOYSA-N
Formula:	C24H46O4
SMILES:	CCCCCCCCCCCCOC(=O)CCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	398.62

Physical Properties

Property code	Value	Unit	Source
gf	-323.96	kJ/mol	Joback Method
hf	-1044.13	kJ/mol	Joback Method
hfus	52.92	kJ/mol	Joback Method
hvap	86.17	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.845		Crippen Method
mcvol	363.900	ml/mol	McGowan Method
pc	862.01	kPa	Joback Method
rinsol	2601.00		NIST Webbook
tb	899.78	K	Joback Method
tc	1101.76	K	Joback Method
tf	459.56	K	Joback Method
vc	1.409	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1218.83	J/molxK	899.78	Joback Method
cpg	1238.81	J/molxK	933.44	Joback Method
cpg	1257.37	J/molxK	967.11	Joback Method
cpg	1274.54	J/molxK	1000.77	Joback Method
cpg	1290.36	J/molxK	1034.43	Joback Method
cpg	1304.87	J/molxK	1068.10	Joback Method
cpg	1318.09	J/molxK	1101.76	Joback Method
dvisc	0.0008558	Paxs	459.56	Joback Method
dvisc	0.0003072	Paxs	532.93	Joback Method

dvisc	0.0001413	Paxs	606.30	Joback Method
dvisc	0.0000768	Paxs	679.67	Joback Method
dvisc	0.0000471	Paxs	753.04	Joback Method
dvisc	0.0000314	Paxs	826.41	Joback Method
dvisc	0.0000224	Paxs	899.78	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U349365&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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