

Adipic acid, dodecyl 3-oxobut-2-yl ester

Inchi:	InChI=1S/C22H40O5/c1-4-5-6-7-8-9-10-11-12-15-18-26-21(24)16-13-14-17-22(25)27-20
InchiKey:	RDBHJOPVLWFEQZ-UHFFFAOYSA-N
Formula:	C22H40O5
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	384.55

Physical Properties

Property code	Value	Unit	Source
gf	-464.84	kJ/mol	Joback Method
hf	-1104.87	kJ/mol	Joback Method
hfus	56.39	kJ/mol	Joback Method
hvap	89.24	kJ/mol	Joback Method
log10ws	-6.15		Crippen Method
logp	5.532		Crippen Method
mvol	337.290	ml/mol	McGowan Method
pc	997.02	kPa	Joback Method
rinpol	2633.00		NIST Webbook
rinpol	2633.00		NIST Webbook
tb	908.77	K	Joback Method
tc	1112.66	K	Joback Method
tf	516.95	K	Joback Method
vc	1.315	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1114.67	J/molxK	908.77	Joback Method
cpg	1189.62	J/molxK	1078.68	Joback Method
cpg	1177.19	J/molxK	1044.70	Joback Method
cpg	1163.50	J/molxK	1010.72	Joback Method
cpg	1148.54	J/molxK	976.73	Joback Method
cpg	1132.27	J/molxK	942.75	Joback Method
cpg	1200.82	J/molxK	1112.66	Joback Method
dvisc	0.0000342	Paxs	908.77	Joback Method

dvisc	0.0000457	Paxs	843.47	Joback Method
dvisc	0.0000641	Paxs	778.16	Joback Method
dvisc	0.0000957	Paxs	712.86	Joback Method
dvisc	0.0001549	Paxs	647.56	Joback Method
dvisc	0.0002793	Paxs	582.25	Joback Method
dvisc	0.0005844	Paxs	516.95	Joback Method

Sources

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=U353756&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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