

Sebacic acid, nonyl 3-oxobut-2-yl ester

Inchi:	InChI=1S/C23H42O5/c1-4-5-6-7-10-13-16-19-27-22(25)17-14-11-8-9-12-15-18-23(26)28
InchiKey:	PINYLBZBQIINVQQ-UHFFFAOYSA-N
Formula:	C23H42O5
SMILES:	CCCCCCCCCOC(=O)CCCCCCCCC(=O)OC(C)C(C)=O
Mol. weight [g/mol]:	398.58

Physical Properties

Property code	Value	Unit	Source
gf	-456.42	kJ/mol	Joback Method
hf	-1125.51	kJ/mol	Joback Method
hfus	58.98	kJ/mol	Joback Method
hvap	91.46	kJ/mol	Joback Method
log10ws	-6.57		Crippen Method
logp	5.922		Crippen Method
mcvol	351.380	ml/mol	McGowan Method
pc	939.22	kPa	Joback Method
rinqol	2751.00		NIST Webbook
tb	931.65	K	Joback Method
tc	1141.56	K	Joback Method
tf	528.22	K	Joback Method
vc	1.371	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1176.67	J/molxK	931.65	Joback Method
cpg	1194.68	J/molxK	966.64	Joback Method
cpg	1211.25	J/molxK	1001.62	Joback Method
cpg	1226.41	J/molxK	1036.61	Joback Method
cpg	1240.19	J/molxK	1071.59	Joback Method
cpg	1252.63	J/molxK	1106.58	Joback Method
cpg	1263.75	J/molxK	1141.56	Joback Method
dvisc	0.0005155	Paxs	528.22	Joback Method
dvisc	0.0002441	Paxs	595.46	Joback Method

dvisc	0.0001345	Paxs	662.70	Joback Method
dvisc	0.0000828	Paxs	729.93	Joback Method
dvisc	0.0000552	Paxs	797.17	Joback Method
dvisc	0.0000393	Paxs	864.41	Joback Method
dvisc	0.0000293	Paxs	931.65	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=U355781&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
mccvol:	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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