

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

Inchi:	InChI=1S/C30H58O4/c1-6-7-8-9-10-11-12-13-16-19-22-25-33-28(31)23-20-17-14-15-18-
InchiKey:	BMEMCULPXWNKSY-UHFFFAOYSA-N
Formula:	C30H58O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCCCCCC(=O)OC(C(C)C)C(C)C
Mol. weight [g/mol]:	482.78

Physical Properties

Property code	Value	Unit	Source
gf	-273.44	kJ/mol	Joback Method
hf	-1167.97	kJ/mol	Joback Method
hfus	68.46	kJ/mol	Joback Method
hvap	99.52	kJ/mol	Joback Method
log10ws	-9.73		Crippen Method
logp	9.185		Crippen Method
mcvol	448.440	ml/mol	McGowan Method
pc	630.66	kPa	Joback Method
rinpol	3230.00		NIST Webbook
tb	1037.06	K	Joback Method
tc	1294.33	K	Joback Method
tf	527.18	K	Joback Method
vc	1.746	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1605.81	J/molxK	1037.06	Joback Method
cpg	1629.04	J/molxK	1079.94	Joback Method
cpg	1649.85	J/molxK	1122.82	Joback Method
cpg	1668.35	J/molxK	1165.70	Joback Method
cpg	1684.64	J/molxK	1208.58	Joback Method
cpg	1698.82	J/molxK	1251.45	Joback Method
cpg	1711.00	J/molxK	1294.33	Joback Method
dvisc	0.0003531	Paxs	527.18	Joback Method
dvisc	0.0001236	Paxs	612.16	Joback Method

dvisc	0.0000559	Paxs	697.14	Joback Method
dvisc	0.0000300	Paxs	782.12	Joback Method
dvisc	0.0000182	Paxs	867.10	Joback Method
dvisc	0.0000121	Paxs	952.08	Joback Method
dvisc	0.0000086	Paxs	1037.06	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=U355435&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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