

Sebacic acid, 3-methylphenyl undecyl ester

Inchi:	InChI=1S/C28H46O4/c1-3-4-5-6-7-8-11-14-17-23-31-27(29)21-15-12-9-10-13-16-22-28(30)
InchiKey:	ODQBZBZHXFDMMN-UHFFFAOYSA-N
Formula:	C28H46O4
SMILES:	CCCCCCCCCOC(=O)CCCCCCCC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	446.66

Physical Properties

Property code	Value	Unit	Source
gf	-180.18	kJ/mol	Joback Method
hf	-885.79	kJ/mol	Joback Method
hfus	67.50	kJ/mol	Joback Method
hvap	99.17	kJ/mol	Joback Method
log10ws	-9.08		Crippen Method
logp	8.095		Crippen Method
mvol	396.500	ml/mol	McGowan Method
pc	817.26	kPa	Joback Method
rinpol	3381.00		NIST Webbook
tb	1024.28	K	Joback Method
tc	1259.00	K	Joback Method
tf	588.58	K	Joback Method
vc	1.544	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.60	J/molxK	1024.28	Joback Method
cpg	1387.84	J/molxK	1063.40	Joback Method
cpg	1404.30	J/molxK	1102.52	Joback Method
cpg	1419.05	J/molxK	1141.64	Joback Method
cpg	1432.16	J/molxK	1180.76	Joback Method
cpg	1443.70	J/molxK	1219.88	Joback Method
cpg	1453.73	J/molxK	1259.00	Joback Method
dvisc	0.0002368	Paxs	588.58	Joback Method
dvisc	0.0001195	Paxs	661.20	Joback Method

dvisc	0.0000690	Paxs	733.81	Joback Method
dvisc	0.0000440	Paxs	806.43	Joback Method
dvisc	0.0000302	Paxs	879.05	Joback Method
dvisc	0.0000220	Paxs	951.66	Joback Method
dvisc	0.0000167	Paxs	1024.28	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=U354933&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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