

Sebacic acid, 3,5-dimethylphenyl octyl ester

Inchi:	InChI=1S/C26H42O4/c1-4-5-6-7-12-15-18-29-25(27)16-13-10-8-9-11-14-17-26(28)30-24
InchiKey:	LNOLUBQDBHQFY-UHFFFAOYSA-N
Formula:	C26H42O4
SMILES:	CCCCCCCCOC(=O)CCCCCCCC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]:	418.61

Physical Properties

Property code	Value	Unit	Source
gf	-206.65	kJ/mol	Joback Method
hf	-855.98	kJ/mol	Joback Method
hfus	61.93	kJ/mol	Joback Method
hvap	95.38	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.233		Crippen Method
mvol	368.320	ml/mol	McGowan Method
pc	906.70	kPa	Joback Method
rinpol	3148.00		NIST Webbook
tb	983.50	K	Joback Method
tc	1204.69	K	Joback Method
tf	578.56	K	Joback Method
vc	1.431	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1243.12	J/molxK	983.50	Joback Method
cpg	1260.57	J/molxK	1020.37	Joback Method
cpg	1276.44	J/molxK	1057.23	Joback Method
cpg	1290.78	J/molxK	1094.10	Joback Method
cpg	1303.62	J/molxK	1130.96	Joback Method
cpg	1315.02	J/molxK	1167.83	Joback Method
cpg	1325.02	J/molxK	1204.69	Joback Method
dvisc	0.0002672	Paxs	578.56	Joback Method
dvisc	0.0001440	Paxs	646.05	Joback Method

dvisc	0.0000872	Paxs	713.54	Joback Method
dvisc	0.0000576	Paxs	781.03	Joback Method
dvisc	0.0000406	Paxs	848.52	Joback Method
dvisc	0.0000302	Paxs	916.01	Joback Method
dvisc	0.0000233	Paxs	983.50	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=U354596&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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