

Sebacic acid, 3,5-dimethylphenyl hexyl ester

Inchi:	InChI=1S/C24H38O4/c1-4-5-6-13-16-27-23(25)14-11-9-7-8-10-12-15-24(26)28-22-18-20
InchiKey:	AINZRRCXHISHJO-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCCCOC(=O)CCCCCCCC(=O)Oc1cc(C)cc(C)c1
Mol. weight [g/mol]:	390.56

Physical Properties

Property code	Value	Unit	Source
gf	-223.49	kJ/mol	Joback Method
hf	-814.70	kJ/mol	Joback Method
hfus	56.75	kJ/mol	Joback Method
hvap	90.93	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.453		Crippen Method
mvol	340.140	ml/mol	McGowan Method
pc	1021.38	kPa	Joback Method
rinpol	2941.00		NIST Webbook
tb	937.74	K	Joback Method
tc	1148.48	K	Joback Method
tf	556.02	K	Joback Method
vc	1.319	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1118.89	J/molxK	937.74	Joback Method
cpg	1135.82	J/molxK	972.86	Joback Method
cpg	1151.36	J/molxK	1007.99	Joback Method
cpg	1165.54	J/molxK	1043.11	Joback Method
cpg	1178.40	J/molxK	1078.24	Joback Method
cpg	1189.97	J/molxK	1113.36	Joback Method
cpg	1200.28	J/molxK	1148.48	Joback Method
dvisc	0.0003364	Paxs	556.02	Joback Method
dvisc	0.0001850	Paxs	619.64	Joback Method

dvisc	0.0001137	Paxs	683.26	Joback Method
dvisc	0.0000760	Paxs	746.88	Joback Method
dvisc	0.0000540	Paxs	810.50	Joback Method
dvisc	0.0000404	Paxs	874.12	Joback Method
dvisc	0.0000314	Paxs	937.74	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=U354594&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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