

Sebacic acid, 3,5-dimethylphenyl isoheptyl ester

Inchi:	InChI=1S/C24H38O4/c1-19(2)12-11-15-27-23(25)13-9-7-5-6-8-10-14-24(26)28-22-17-20
InchiKey:	DXAUWUNVMYEGEH-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	<chem>Cc1cc(C)cc(OC(=O)CCCCCCCC(=O)OCCCC(C)C)c1</chem>
Mol. weight [g/mol]:	390.56

Physical Properties

Property code	Value	Unit	Source
gf	-225.93	kJ/mol	Joback Method
hf	-819.98	kJ/mol	Joback Method
hfus	53.23	kJ/mol	Joback Method
hvap	90.54	kJ/mol	Joback Method
log10ws	-7.22		Crippen Method
logp	6.309		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1026.63	kPa	Joback Method
rinsol	2891.00		NIST Webbook
tb	937.30	K	Joback Method
tc	1148.38	K	Joback Method
tf	541.02	K	Joback Method
vc	1.313	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.31	J/molxK	937.30	Joback Method
cpg	1136.23	J/molxK	972.48	Joback Method
cpg	1151.74	J/molxK	1007.66	Joback Method
cpg	1165.88	J/molxK	1042.84	Joback Method
cpg	1178.68	J/molxK	1078.02	Joback Method
cpg	1190.17	J/molxK	1113.20	Joback Method
cpg	1200.39	J/molxK	1148.38	Joback Method
dvisc	0.0003707	Paxs	541.02	Joback Method
dvisc	0.0001919	Paxs	607.07	Joback Method

dvisc	0.0001130	Paxs	673.11	Joback Method
dvisc	0.0000732	Paxs	739.16	Joback Method
dvisc	0.0000509	Paxs	805.21	Joback Method
dvisc	0.0000374	Paxs	871.25	Joback Method
dvisc	0.0000287	Paxs	937.30	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354593&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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