

Sebacic acid, heptyl 3-methylphenyl ester

Inchi:	InChI=1S/C24H38O4/c1-3-4-5-10-13-19-27-23(25)17-11-8-6-7-9-12-18-24(26)28-22-16-
InchiKey:	GMPKTLRBKKKJQS-UHFFFAOYSA-N
Formula:	C24H38O4
SMILES:	CCCCCCCOC(=O)CCCCCCCC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]:	390.56

Physical Properties

Property code	Value	Unit	Source
gf	-213.86	kJ/mol	Joback Method
hf	-803.23	kJ/mol	Joback Method
hfus	57.14	kJ/mol	Joback Method
hvap	90.27	kJ/mol	Joback Method
log10ws	-7.40		Crippen Method
logp	6.535		Crippen Method
mcvol	340.140	ml/mol	McGowan Method
pc	1031.25	kPa	Joback Method
rinsol	2963.00		NIST Webbook
tb	932.76	K	Joback Method
tc	1142.45	K	Joback Method
tf	543.50	K	Joback Method
vc	1.319	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1119.44	J/molxK	932.76	Joback Method
cpg	1136.46	J/molxK	967.71	Joback Method
cpg	1152.13	J/molxK	1002.66	Joback Method
cpg	1166.46	J/molxK	1037.60	Joback Method
cpg	1179.51	J/molxK	1072.55	Joback Method
cpg	1191.30	J/molxK	1107.50	Joback Method
cpg	1201.88	J/molxK	1142.45	Joback Method
dvisc	0.0003848	Paxs	543.50	Joback Method
dvisc	0.0002018	Paxs	608.38	Joback Method

dvisc	0.0001199	Paxs	673.25	Joback Method
dvisc	0.0000780	Paxs	738.13	Joback Method
dvisc	0.0000544	Paxs	803.01	Joback Method
dvisc	0.0000401	Paxs	867.88	Joback Method
dvisc	0.0000308	Paxs	932.76	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354929&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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