Sebacic acid, 3-methylphenyl octyl ester

Inchi: InChI=1S/C25H40O4/c1-3-4-5-6-11-14-20-28-24(26)18-12-9-7-8-10-13-19-25(27)29-23-1
InchiKey: LLASFIGGWUYVGP-UHFFFAOYSA-N
Formula: C25H40O4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cccc(C)c1
Mol. weight [g/mol]: 404.58

Physical Properties

Property code	Value	Unit	Source
gf	-205.44	kJ/mol	Joback Method
hf	-823.87	kJ/mol	Joback Method
hfus	59.73	kJ/mol	Joback Method
hvap	92.49	kJ/mol	Joback Method
log10ws	-7.82		Crippen Method
logp	6.925		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	970.49	kPa	Joback Method
rinpol	3069.00		NIST Webbook
tb	955.64	K	Joback Method
tc	1169.97	K	Joback Method
tf	554.77	K	Joback Method
vc	1.375	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1181.32	J/mol×K	955.64	Joback Method
cpg	1253.73	J/mol×K	1134.25	Joback Method
cpg	1241.97	J/mol×K	1098.53	Joback Method
cpg	1228.89	J/mol×K	1062.81	Joback Method
cpg	1214.46	J/mol×K	1027.08	Joback Method
cpg	1198.61	J/mol×K	991.36	Joback Method
cpg	1264.21	J/mol×K	1169.97	Joback Method
dvisc	0.0000265	Pa×s	955.64	Joback Method
dvisc	0.0000346	Pa×s	888.83	Joback Method

dvisc	0.0000471	Pa×s	822.02	Joback Method
dvisc	0.0000678	Pa×s	755.20	Joback Method
dvisc	0.0001048	Pa×s	688.39	Joback Method
dvisc	0.0001777	Pa×s	621.58	Joback Method
dvisc	0.0003423	Pa×s	554.77	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=U354930&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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