Sebacic acid, hexyl 3-propylphenyl ester

Inchi: InChI=1S/C25H40O4/c1-3-5-6-15-21-28-24(26)19-11-9-7-8-10-12-20-25(27)29-23-18-14
InchiKey: XEFHEKVLLSFDGU-UHFFFAOYSA-N
Formula: C25H40O4
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1CCC
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	-7.73		Crippen Method
logp	6.789		Crippen Method
mcvol	354.230	ml/mol	McGowan Method
pc	970.49	kPa	Joback Method
rinpol	2926.00		NIST Webbook
rinpol	2926.00		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	1198.61	J/mol×K	991.36	Joback Method
cpg	1214.46	J/mol×K	1027.08	Joback Method
cpg	1228.89	J/mol×K	1062.81	Joback Method
cpg	1241.97	J/mol×K	1098.53	Joback Method
cpg	1253.73	J/mol×K	1134.25	Joback Method
cpg	1264.21	J/mol×K	1169.97	Joback Method
dvisc	0.0003423	Pa×s	554.77	Joback Method

dvisc	0.0001777	Pa×s	621.58	Joback Method
dvisc	0.0001048	Pa×s	688.39	Joback Method
dvisc	0.0000678	Pa×s	755.20	Joback Method
dvisc	0.0000471	Pa×s	822.02	Joback Method
dvisc	0.0000346	Pa×s	888.83	Joback Method
dvisc	0.0000265	Pa×s	955.64	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355054&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Latest version available from:
https://www.chemeo.com/cid/12-695-7/Sebacic-acid-hexyl-3-propylphenyl-ester.pdf
Generated by Cheméo on 2024-10-12 09:13:41.705211539 +0000 UTC m=+3305284.342180791.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.