Sebacic acid, hexyl 4-isopropoxyphenyl ester

Inchi: InChI=1S/C25H40O5/c1-4-5-6-13-20-28-24(26)14-11-9-7-8-10-12-15-25(27)30-23-18-16
InchiKey: PVYAKQAULGFOSX-UHFFFAOYSA-N
Formula: C25H40O5
SMILES: CCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(OC(C)C)cc1
Mol. weight [g/mol]: 420.58

Physical Properties

Property code	Value	Unit	Source
gf	-312.88	kJ/mol	Joback Method
hf	-961.37	kJ/mol	Joback Method
hfus	57.40	kJ/mol	Joback Method
hvap	94.52	kJ/mol	Joback Method
log10ws	-7.58		Crippen Method
logp	6.623		Crippen Method
mcvol	360.100	ml/mol	McGowan Method
pc	965.07	kPa	Joback Method
rinpol	3016.00		NIST Webbook
rinpol	3016.00		NIST Webbook
tb	977.62	K	Joback Method
tc	1197.02	K	Joback Method
tf	562.00	K	Joback Method
vc	1.387	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1211.31	J/mol×K	977.62	Joback Method
cpg	1277.64	J/mol×K	1160.45	Joback Method
cpg	1267.55	J/mol×K	1123.89	Joback Method
cpg	1255.91	J/mol×K	1087.32	Joback Method
cpg	1242.67	J/mol×K	1050.75	Joback Method
cpg	1227.82	J/mol×K	1014.19	Joback Method
cpg	1286.20	J/mol×K	1197.02	Joback Method
dvisc	0.0000178	Pa×s	977.62	Joback Method

dvisc	0.0000235	Pa×s	908.35	Joback Method
dvisc	0.0000324	Pa×s	839.08	Joback Method
dvisc	0.0000474	Pa×s	769.81	Joback Method
dvisc	0.0000747	Pa×s	700.54	Joback Method
dvisc	0.0001302	Pa×s	631.27	Joback Method
dvisc	0.0002600	Pa×s	562.00	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354407&Units=SI

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