Sebacic acid, 2-methylphenyl undecyl ester

Inchi: InChI=1S/C28H46O4/c1-3-4-5-6-7-8-11-14-19-24-31-27(29)22-15-12-9-10-13-16-23-28(3
InchiKey: UEKSSMPIEYRNAB-UHFFFAOYSA-N
Formula: C28H46O4
SMILES: CCCCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccccc1C
Mol. weight [g/mol]: 446.66

Physical Properties

Property code	Value	Unit	Source
gf	-180.18	kJ/mol	Joback Method
hf	-885.79	kJ/mol	Joback Method
hfus	67.50	kJ/mol	Joback Method
hvap	99.17	kJ/mol	Joback Method
log10ws	-9.08		Crippen Method
logp	8.095		Crippen Method
mcvol	396.500	ml/mol	McGowan Method
pc	817.26	kPa	Joback Method
rinpol	3371.00		NIST Webbook
tb	1024.28	K	Joback Method
tc	1259.00	K	Joback Method
tf	588.58	K	Joback Method
vc	1.544	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1369.60	J/mol×K	1024.28	Joback Method
cpg	1387.84	J/mol×K	1063.40	Joback Method
cpg	1404.30	J/mol×K	1102.52	Joback Method
cpg	1419.05	J/mol×K	1141.64	Joback Method
cpg	1432.16	J/mol×K	1180.76	Joback Method
cpg	1443.70	J/mol×K	1219.88	Joback Method
cpg	1453.73	J/mol×K	1259.00	Joback Method
dvisc	0.0002368	Pa×s	588.58	Joback Method
dvisc	0.0001195	Pa×s	661.20	Joback Method

dvisc	0.0000690	Pa×s	733.81	Joback Method
dvisc	0.0000440	Pa×s	806.43	Joback Method
dvisc	0.0000302	Pa×s	879.05	Joback Method
dvisc	0.0000220	Pa×s	951.66	Joback Method
dvisc	0.0000167	Pa×s	1024.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354381&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

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