Sebacic acid, 2-chlorophenethyl octyl ester

Inchi: InChI=1S/C26H41ClO4/c1-2-3-4-5-10-15-21-30-25(28)18-11-8-6-7-9-12-19-26(29)31-22-
InchiKey: KQGMJYCTLCLXOP-UHFFFAOYSA-N
Formula: C26H41ClO4
SMILES: CCCCCCCCOC(=O)CCCCCCCCC(=O)OCCc1ccccc1Cl
Mol. weight [g/mol]: 453.05

Physical Properties

Property code	Value	Unit	Source
gf	-208.95	kJ/mol	Joback Method
hf	-860.25	kJ/mol	Joback Method
hfus	66.52	kJ/mol	Joback Method
hvap	99.10	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	7.450		Crippen Method
mcvol	380.560	ml/mol	McGowan Method
pc	894.80	kPa	Joback Method
rinpol	3141.00		NIST Webbook
rinpol	3141.00		NIST Webbook
tb	1015.95	K	Joback Method
tc	1245.61	K	Joback Method
tf	595.96	K	Joback Method
vc	1.480	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1269.77	J/mol×K	1015.95	Joback Method
cpg	1336.48	J/mol×K	1207.34	Joback Method
cpg	1326.09	J/mol×K	1169.06	Joback Method
cpg	1314.29	J/mol×K	1130.78	Joback Method
cpg	1301.01	J/mol×K	1092.50	Joback Method
cpg	1286.19	J/mol×K	1054.23	Joback Method
cpg	1345.50	J/mol×K	1245.61	Joback Method
dvisc	0.0000191	Pa×s	1015.95	Joback Method

dvisc	0.0000249	Pa×s	945.95	Joback Method
dvisc	0.0000339	Pa×s	875.95	Joback Method
dvisc	0.0000486	Pa×s	805.95	Joback Method
dvisc	0.0000748	Pa×s	735.96	Joback Method
dvisc	0.0001260	Pa×s	665.96	Joback Method
dvisc	0.0002398	Pa×s	595.96	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U416232&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