Sebacic acid, 4-chloro-2-methylbenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C25H39ClO4/c1-5-12-23(19(2)3)30-25(28)14-11-9-7-6-8-10-13-24(27)29-18-21

InchiKey: GOOZTEHCOAISLS-UHFFFAOYSA-N

Formula: C25H39ClO4

SMILES: CCCC(OC(=O)CCCCCCCCC(=O)OCc1ccc(Cl)cc1C)C(C)C

Mol. weight [g/mol]: 439.03

Physical Properties

Property code	Value	Unit	Source
gf	-231.88	kJ/mol	Joback Method
hf	-861.64	kJ/mol	Joback Method
hfus	56.49	kJ/mol	Joback Method
hvap	96.77	kJ/mol	Joback Method
log10ws	-8.22		Crippen Method
logp	7.180		Crippen Method
mcvol	366.470	ml/mol	McGowan Method
pc	949.08	kPa	Joback Method
rinpol	3006.00		NIST Webbook
rinpol	3006.00		NIST Webbook
tb	997.17	K	Joback Method
tc	1220.82	K	Joback Method
tf	567.21	K	Joback Method
vc	1.413	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1207.62	J/mol×K	997.17	Joback Method
cpg	1223.46	J/mol×K	1034.45	Joback Method
cpg	1237.73	J/mol×K	1071.72	Joback Method
cpg	1250.50	J/mol×K	1109.00	Joback Method
cpg	1261.81	J/mol×K	1146.27	Joback Method
cpg	1271.69	J/mol×K	1183.55	Joback Method
cpg	1280.19	J/mol×K	1220.82	Joback Method
dvisc	0.0002873	Pa×s	567.21	Joback Method

dvisc	0.0001416	Pa×s	638.87	Joback Method
dvisc	0.0000805	Pa×s	710.53	Joback Method
dvisc	0.0000507	Pa×s	782.19	Joback Method
dvisc	0.0000346	Pa×s	853.85	Joback Method
dvisc	0.0000250	Pa×s	925.51	Joback Method
dvisc	0.0000189	Pa×s	997.17	Joback Method

Sources

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=U380589&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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