Sebacic acid, 2-methylhex-3-yl 2,4,6-trichlorobenzyl ester

Inchi: InChI=1S/C24H35Cl3O4/c1-4-11-22(17(2)3)31-24(29)13-10-8-6-5-7-9-12-23(28)30-16-19

InchiKey: LCDIFUCTVCODHF-UHFFFAOYSA-N

Formula: C24H35Cl3O4

SMILES: CCCC(OC(=O)CCCCCCCCC(=O)OCc1c(Cl)cc(Cl)cc1Cl)C(C)C

Mol. weight [g/mol]: 493.89

Physical Properties

Property code	Value	Unit	Source
gf	-273.79	kJ/mol	Joback Method
hf	-883.95	kJ/mol	Joback Method
hfus	61.91	kJ/mol	Joback Method
hvap	103.97	kJ/mol	Joback Method
log10ws	-9.12		Crippen Method
logp	8.179		Crippen Method
mcvol	376.860	ml/mol	McGowan Method
pc	953.19	kPa	Joback Method
rinpol	3147.00		NIST Webbook
rinpol	3147.00		NIST Webbook
tb	1054.13	K	Joback Method
tc	1290.92	K	Joback Method
tf	628.30	K	Joback Method
vc	1.454	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1191.21	J/mol×K	1054.13	Joback Method
cpg	1240.27	J/mol×K	1251.45	Joback Method
cpg	1233.48	J/mol×K	1211.99	Joback Method
cpg	1225.23	J/mol×K	1172.52	Joback Method
cpg	1215.46	J/mol×K	1133.06	Joback Method
cpg	1204.14	J/mol×K	1093.59	Joback Method
cpg	1245.63	J/mol×K	1290.92	Joback Method
dvisc	0.0000157	Pa×s	1054.13	Joback Method

dvisc	0.0000204	Pa×s	983.16	Joback Method
dvisc	0.0000275	Pa×s	912.19	Joback Method
dvisc	0.0000390	Pa×s	841.22	Joback Method
dvisc	0.0000589	Pa×s	770.24	Joback Method
dvisc	0.0000969	Pa×s	699.27	Joback Method
dvisc	0.0001784	Pa×s	628.30	Joback Method

Sources

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=U380576&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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