Sebacic acid, 2,5-dichlorobenzyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C24H36Cl2O4/c1-4-11-22(18(2)3)30-24(28)13-10-8-6-5-7-9-12-23(27)29-17-19

InchiKey: ZPMZTWOYEMTGKZ-UHFFFAOYSA-N

Formula: C24H36Cl2O4

SMILES: CCCC(OC(=O)CCCCCCCCC(=O)OCc1cc(Cl)ccc1Cl)C(C)C

Mol. weight [g/mol]: 459.45

Physical Properties

Property code	Value	Unit	Source
gf	-252.23	kJ/mol	Joback Method
hf	-856.74	kJ/mol	Joback Method
hfus	58.10	kJ/mol	Joback Method
hvap	98.92	kJ/mol	Joback Method
log10ws	-8.43		Crippen Method
logp	7.525		Crippen Method
mcvol	364.620	ml/mol	McGowan Method
pc	984.55	kPa	Joback Method
rinpol	3062.00		NIST Webbook
rinpol	3062.00		NIST Webbook
tb	1011.72	K	Joback Method
tc	1238.63	K	Joback Method
tf	585.86	K	Joback Method
vc	1.405	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1170.34	J/mol×K	1011.72	Joback Method
cpg	1184.73	J/mol×K	1049.54	Joback Method
cpg	1197.62	J/mol×K	1087.36	Joback Method
cpg	1209.04	J/mol×K	1125.18	Joback Method
cpg	1219.04	J/mol×K	1162.99	Joback Method
cpg	1227.67	J/mol×K	1200.81	Joback Method
cpg	1234.96	J/mol×K	1238.63	Joback Method
dvisc	0.0002552	Pa×s	585.86	Joback Method

dvisc	0.0001300	Pa×s	656.84	Joback Method
dvisc	0.0000756	Pa×s	727.81	Joback Method
dvisc	0.0000484	Pa×s	798.79	Joback Method
dvisc	0.0000333	Pa×s	869.77	Joback Method
dvisc	0.0000242	Pa×s	940.74	Joback Method
dvisc	0.0000185	Pa×s	1011.72	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=U380615&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

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