Sebacic acid, 2,4-dichlorophenethyl heptyl ester

Inchi: InChI=1S/C25H38Cl2O4/c1-2-3-4-9-12-18-30-24(28)13-10-7-5-6-8-11-14-25(29)31-19-17

InchiKey: HROZXJMEQBWTPK-UHFFFAOYSA-N

Formula: C25H38Cl2O4

SMILES: CCCCCCCOC(=O)CCCCCCCCC(=O)OCCc1ccc(Cl)cc1Cl

Mol. weight [g/mol]: 473.47

Physical Properties

Property code	Value	Unit	Source
gf	-238.93	kJ/mol	Joback Method
hf	-866.82	kJ/mol	Joback Method
hfus	67.74	kJ/mol	Joback Method
hvap	101.93	kJ/mol	Joback Method
log10ws	-8.49		Crippen Method
logp	7.713		Crippen Method
mcvol	378.710	ml/mol	McGowan Method
pc	918.83	kPa	Joback Method
rinpol	3117.00		NIST Webbook
rinpol	3117.00		NIST Webbook
tb	1035.48	K	Joback Method
tc	1269.32	K	Joback Method
tf	627.13	K	Joback Method
vc	1.474	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1230.98	J/mol×K	1035.48	Joback Method
cpg	1245.78	J/mol×K	1074.45	Joback Method
cpg	1258.99	J/mol×K	1113.43	Joback Method
cpg	1270.66	J/mol×K	1152.40	Joback Method
cpg	1280.85	J/mol×K	1191.37	Joback Method
cpg	1289.61	J/mol×K	1230.35	Joback Method
cpg	1297.00	J/mol×K	1269.32	Joback Method
dvisc	0.0001925	Pa×s	627.13	Joback Method

dvisc	0.0001085	Pa×s	695.19	Joback Method
dvisc	0.0000677	Pa×s	763.25	Joback Method
dvisc	0.0000456	Pa×s	831.31	Joback Method
dvisc	0.0000327	Pa×s	899.36	Joback Method
dvisc	0.0000245	Pa×s	967.42	Joback Method
dvisc	0.0000191	Pa×s	1035.48	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=U416821&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