

Sebacic acid, di(2,6-dichlorophenyl) ester

Inchi: InChI=1S/C22H22Cl4O4/c23-15-9-7-10-16(24)21(15)29-19(27)13-5-3-1-2-4-6-14-20(28)
InchiKey: PPXICGKGQXNXGS-UHFFFAOYSA-N
Formula: C22H22Cl4O4
SMILES: O=C(CCCCCCCC(=O)Oc1c(Cl)cccc1Cl)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 492.22

Physical Properties

Property code	Value	Unit	Source
gf	-194.90	kJ/mol	Joback Method
hf	-622.79	kJ/mol	Joback Method
hfus	61.62	kJ/mol	Joback Method
hvap	107.62	kJ/mol	Joback Method
log10ws	-9.00		Crippen Method
logp	7.932		Crippen Method
mvol	337.160	ml/mol	McGowan Method
pc	1290.21	kPa	Joback Method
rinpol	3615.00		NIST Webbook
rinpol	3615.00		NIST Webbook
tb	1078.34	K	Joback Method
tc	1323.43	K	Joback Method
tf	704.62	K	Joback Method
vc	1.296	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	973.58	J/molxK	1078.34	Joback Method
cpg	982.06	J/molxK	1119.19	Joback Method
cpg	989.14	J/molxK	1160.04	Joback Method
cpg	994.87	J/molxK	1200.88	Joback Method
cpg	999.29	J/molxK	1241.73	Joback Method
cpg	1002.44	J/molxK	1282.58	Joback Method
cpg	1004.38	J/molxK	1323.43	Joback Method
dvisc	0.0001418	Paxs	704.62	Joback Method

dvisc	0.0000930	Paxs	766.91	Joback Method
dvisc	0.0000649	Paxs	829.19	Joback Method
dvisc	0.0000477	Paxs	891.48	Joback Method
dvisc	0.0000364	Paxs	953.77	Joback Method
dvisc	0.0000288	Paxs	1016.05	Joback Method
dvisc	0.0000234	Paxs	1078.34	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=U354883&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_cvol:	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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