

Sebacic acid, ethyl 2,3,4,5-tetrachlorophenyl ester

Inchi:	InChI=1S/C18H22Cl4O4/c1-2-25-14(23)9-7-5-3-4-6-8-10-15(24)26-13-11-12(19)16(20)18
InchiKey:	BYXCBDULMSLGNN-UHFFFAOYSA-N
Formula:	C18H22Cl4O4
SMILES:	CCOC(=O)CCCCCCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]:	444.18

Physical Properties

Property code	Value	Unit	Source
gf	-340.99	kJ/mol	Joback Method
hf	-776.76	kJ/mol	Joback Method
hfus	57.22	kJ/mol	Joback Method
hvap	96.44	kJ/mol	Joback Method
log10ws	-7.57		Crippen Method
logp	6.889		Crippen Method
mvol	304.560	ml/mol	McGowan Method
pc	1340.78	kPa	Joback Method
rinpol	2990.00		NIST Webbook
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tb	960.14	K	Joback Method
tc	1181.98	K	Joback Method
tf	633.12	K	Joback Method
vc	1.179	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	853.87	J/molxK	960.14	Joback Method
cpg	864.61	J/molxK	997.11	Joback Method
cpg	874.18	J/molxK	1034.09	Joback Method
cpg	882.58	J/molxK	1071.06	Joback Method
cpg	889.83	J/molxK	1108.03	Joback Method
cpg	895.95	J/molxK	1145.00	Joback Method
cpg	900.93	J/molxK	1181.98	Joback Method
dvisc	0.0002379	Paxs	633.12	Joback Method

dvisc	0.0001583	Paxs	687.62	Joback Method
dvisc	0.0001118	Paxs	742.13	Joback Method
dvisc	0.0000828	Paxs	796.63	Joback Method
dvisc	0.0000637	Paxs	851.13	Joback Method
dvisc	0.0000506	Paxs	905.64	Joback Method
dvisc	0.0000413	Paxs	960.14	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U355286&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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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