

Sebacic acid, octyl 2,4,6-trichlorophenyl ester

Inchi:	InChI=1S/C24H35Cl3O4/c1-2-3-4-5-10-13-16-30-22(28)14-11-8-6-7-9-12-15-23(29)31-24
InchiKey:	MRQWWOQISOSNSB-UHFFFAOYSA-N
Formula:	C24H35Cl3O4
SMILES:	CCCCCCCCOC(=O)CCCCCCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	493.89

Physical Properties

Property code	Value	Unit	Source
gf	-268.91	kJ/mol	Joback Method
hf	-873.39	kJ/mol	Joback Method
hfus	68.95	kJ/mol	Joback Method
hvap	104.75	kJ/mol	Joback Method
log10ws	-9.40		Crippen Method
logp	8.577		Crippen Method
mcvol	376.860	ml/mol	McGowan Method
pc	943.84	kPa	Joback Method
rinqol	3356.00		NIST Webbook
tb	1055.01	K	Joback Method
tc	1293.03	K	Joback Method
tf	658.30	K	Joback Method
vc	1.466	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.69	J/molxK	1055.01	Joback Method
cpg	1241.10	J/molxK	1253.36	Joback Method
cpg	1234.01	J/molxK	1213.69	Joback Method
cpg	1225.47	J/molxK	1174.02	Joback Method
cpg	1215.43	J/molxK	1134.35	Joback Method
cpg	1203.86	J/molxK	1094.68	Joback Method
cpg	1246.79	J/molxK	1293.03	Joback Method
dvisc	0.0000191	Paxs	1055.01	Joback Method
dvisc	0.0000241	Paxs	988.89	Joback Method

dvisc	0.0000316	Paxs	922.77	Joback Method
dvisc	0.0000430	Paxs	856.65	Joback Method
dvisc	0.0000617	Paxs	790.54	Joback Method
dvisc	0.0000946	Paxs	724.42	Joback Method
dvisc	0.0001581	Paxs	658.30	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=U355082&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
mccvol:	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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