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

Inchi: InChI=1S/C25H37Cl3O4/c1-2-3-4-5-8-11-14-17-31-23(29)15-12-9-6-7-10-13-16-24(30)32
InchiKey: VNNXOGYVFOSSOY-UHFFFAOYSA-N
Formula: C25H37Cl3O4
SMILES: CCCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 507.92

Physical Properties

Property code	Value	Unit	Source
gf	-260.49	kJ/mol	Joback Method
hf	-894.03	kJ/mol	Joback Method
hfus	71.55	kJ/mol	Joback Method
hvap	106.97	kJ/mol	Joback Method
log10ws	-9.82		Crippen Method
logp	8.967		Crippen Method
mcvol	390.950	ml/mol	McGowan Method
pc	890.54	kPa	Joback Method
rinpol	3466.00		NIST Webbook
rinpol	3466.00		NIST Webbook
tb	1077.89	K	Joback Method
tc	1323.48	K	Joback Method
tf	669.57	K	Joback Method
vc	1.522	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1251.67	J/mol×K	1077.89	Joback Method
cpg	1265.04	J/mol×K	1118.82	Joback Method
cpg	1276.70	J/mol×K	1159.75	Joback Method
cpg	1286.70	J/mol×K	1200.69	Joback Method
cpg	1295.11	J/mol×K	1241.62	Joback Method
cpg	1301.98	J/mol×K	1282.55	Joback Method
cpg	1307.36	J/mol×K	1323.48	Joback Method
dvisc	0.0001395	Pa×s	669.57	Joback Method

dvisc	0.0000827	Pa×s	737.62	Joback Method
dvisc	0.0000536	Pa×s	805.68	Joback Method
dvisc	0.0000371	Pa×s	873.73	Joback Method
dvisc	0.0000271	Pa×s	941.78	Joback Method
dvisc	0.0000207	Pa×s	1009.84	Joback Method
dvisc	0.0000163	Pa×s	1077.89	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=U355083&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
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