Adipic acid, dodecyl 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C24H35Cl3O4/c1-2-3-4-5-6-7-8-9-10-13-16-30-23(28)14-11-12-15-24(29)31-22

InchiKey: LDYWGNVNSYATPC-UHFFFAOYSA-N

Formula: C24H35Cl3O4

SMILES: CCCCCCCCCCCCOC(=O)CCCCC(=O)Oc1cc(Cl)c(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
rinpol	3359.00		NIST Webbook
rinpol	3359.00		NIST Webbook
tb	1055.01	K	Joback Method
tc	1293.03	K	Joback Method
tf	658.30	K	Joback Method
vc	1.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1190.69	J/mol×K	1055.01	Joback Method
cpg	1203.86	J/mol×K	1094.68	Joback Method
cpg	1215.43	J/mol×K	1134.35	Joback Method
cpg	1225.47	J/mol×K	1174.02	Joback Method
cpg	1234.01	J/mol×K	1213.69	Joback Method
cpg	1241.10	J/mol×K	1253.36	Joback Method
cpg	1246.79	J/mol×K	1293.03	Joback Method
dvisc	0.0001581	Pa×s	658.30	Joback Method

dvisc	0.0000946	Pa×s	724.42	Joback Method
dvisc	0.0000617	Pa×s	790.54	Joback Method
dvisc	0.0000430	Pa×s	856.65	Joback Method
dvisc	0.0000316	Pa×s	922.77	Joback Method
dvisc	0.0000241	Pa×s	988.89	Joback Method
dvisc	0.0000191	Pa×s	1055.01	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=U353865&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