

Glutaric acid, 2,3,5,6-tetrachlorophenyl tridecyl ester

Inchi:	InChI=1S/C24H34Cl4O4/c1-2-3-4-5-6-7-8-9-10-11-12-16-31-20(29)14-13-15-21(30)32-24
InchiKey:	UQJFNDHAKNBYQU-UHFFFAOYSA-N
Formula:	C24H34Cl4O4
SMILES:	CCCCCCCCCCCCOC(=O)CCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl
Mol. weight [g/mol]:	528.34

Physical Properties

Property code	Value	Unit	Source
gf	-290.47	kJ/mol	Joback Method
hf	-900.60	kJ/mol	Joback Method
hfus	72.76	kJ/mol	Joback Method
hvap	109.79	kJ/mol	Joback Method
log10ws	-10.09		Crippen Method
logp	9.230		Crippen Method
mcvol	389.100	ml/mol	McGowan Method
pc	914.39	kPa	Joback Method
rinsol	3614.00		NIST Webbook
tb	1097.42	K	Joback Method
tc	1347.10	K	Joback Method
tf	700.74	K	Joback Method
vc	1.516	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1209.22	J/molxK	1097.42	Joback Method
cpg	1220.88	J/molxK	1139.03	Joback Method
cpg	1230.82	J/molxK	1180.65	Joback Method
cpg	1239.09	J/molxK	1222.26	Joback Method
cpg	1245.73	J/molxK	1263.87	Joback Method
cpg	1250.80	J/molxK	1305.49	Joback Method
cpg	1254.34	J/molxK	1347.10	Joback Method
dvisc	0.0001169	Paxs	700.74	Joback Method
dvisc	0.0000731	Paxs	766.85	Joback Method

dvisc	0.0000492	Paxs	832.97	Joback Method
dvisc	0.0000351	Paxs	899.08	Joback Method
dvisc	0.0000262	Paxs	965.19	Joback Method
dvisc	0.0000204	Paxs	1031.31	Joback Method
dvisc	0.0000163	Paxs	1097.42	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359328&Units=SI

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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