Glutaric acid, 2,6-dichlorophenyl dodecyl ester

Inchi: InChI=1S/C23H34Cl2O4/c1-2-3-4-5-6-7-8-9-10-11-18-28-21(26)16-13-17-22(27)29-23-19
InchiKey: SKNOFNLBDUEAAQ-UHFFFAOYSA-N
Formula: C23H34Cl2O4
SMILES: CCCCCCCCCCCCOC(=O)CCCC(=O)Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 445.42

Physical Properties

Property code	Value	Unit	Source
gf	-255.77	kJ/mol	Joback Method
hf	-825.54	kJ/mol	Joback Method
hfus	62.56	kJ/mol	Joback Method
hvap	97.47	kJ/mol	Joback Method
log10ws	-8.30		Crippen Method
logp	7.533		Crippen Method
mcvol	350.530	ml/mol	McGowan Method
pc	1035.90	kPa	Joback Method
rinpol	3175.00		NIST Webbook
rinpol	3175.00		NIST Webbook
tb	989.72	K	Joback Method
tc	1211.74	K	Joback Method
tf	604.59	K	Joback Method
vc	1.361	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1108.77	J/mol×K	989.72	Joback Method
cpg	1123.10	J/mol×K	1026.72	Joback Method
cpg	1136.04	J/mol×K	1063.73	Joback Method
cpg	1147.62	J/mol×K	1100.73	Joback Method
cpg	1157.88	J/mol×K	1137.74	Joback Method
cpg	1166.86	J/mol×K	1174.74	Joback Method
cpg	1174.60	J/mol×K	1211.74	Joback Method
dvisc	0.0002456	Pa×s	604.59	Joback Method

dvisc	0.0001412	Pa×s	668.78	Joback Method
dvisc	0.0000895	Pa×s	732.97	Joback Method
dvisc	0.0000610	Pa×s	797.15	Joback Method
dvisc	0.0000440	Pa×s	861.34	Joback Method
dvisc	0.0000333	Pa×s	925.53	Joback Method
dvisc	0.0000260	Pa×s	989.72	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358839&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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