Glutaric acid, 2-(2,4-dichlorophenyl)ethyl hexyl ester

Inchi: InChI=1S/C19H26Cl2O4/c1-2-3-4-5-12-24-18(22)7-6-8-19(23)25-13-11-15-9-10-16(20)14
InchiKey: VBEDXHFRGYMWMV-UHFFFAOYSA-N
Formula: C19H26Cl2O4
SMILES: CCCCCCOC(=O)CCCC(=O)OCCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 389.31

Physical Properties

Property code	Value	Unit	Source
gf	-289.45	kJ/mol	Joback Method
hf	-742.98	kJ/mol	Joback Method
hfus	52.20	kJ/mol	Joback Method
hvap	88.57	kJ/mol	Joback Method
log10ws	-5.97		Crippen Method
logp	5.373		Crippen Method
mcvol	294.170	ml/mol	McGowan Method
pc	1348.67	kPa	Joback Method
rinpol	2799.00		NIST Webbook
tb	898.20	K	Joback Method
tc	1108.62	K	Joback Method
tf	559.51	K	Joback Method
vc	1.137	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.45	J/mol×K	898.20	Joback Method
cpg	883.95	J/mol×K	933.27	Joback Method
cpg	896.32	J/mol×K	968.34	Joback Method
cpg	907.58	J/mol×K	1003.41	Joback Method
cpg	917.74	J/mol×K	1038.48	Joback Method
cpg	926.82	J/mol×K	1073.55	Joback Method
cpg	934.86	J/mol×K	1108.62	Joback Method
dvisc	0.0003863	Pa×s	559.51	Joback Method
dvisc	0.0002321	Pa×s	615.96	Joback Method

dvisc	0.0001519	Pa×s	672.41	Joback Method
dvisc	0.0001062	Pa×s	728.86	Joback Method
dvisc	0.0000781	Pa×s	785.30	Joback Method
dvisc	0.0000599	Pa×s	841.75	Joback Method
dvisc	0.0000475	Pa×s	898.20	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U377388&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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