Glutaric acid, 2,4,6-trichlorophenyl 2-ethylhexyl ester

Inchi: InChI=1S/C19H25Cl3O4/c1-3-5-7-13(4-2)12-25-17(23)8-6-9-18(24)26-19-15(21)10-14(20

InchiKey: NDKQNOYIYCQLIY-UHFFFAOYSA-N

Formula: C19H25Cl3O4

SMILES: CCCCC(CC)COC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

Mol. weight [g/mol]: 423.76

Physical Properties

Property code	Value	Unit	Source
gf	-313.45	kJ/mol	Joback Method
hf	-775.47	kJ/mol	Joback Method
hfus	52.48	kJ/mol	Joback Method
hvap	93.23	kJ/mol	Joback Method
log10ws	-7.07		Crippen Method
logp	6.482		Crippen Method
mcvol	306.410	ml/mol	McGowan Method
pc	1306.12	kPa	Joback Method
rinpol	2729.00		NIST Webbook
rinpol	2729.00		NIST Webbook
tb	940.17	K	Joback Method
tc	1158.38	K	Joback Method
tf	586.95	K	Joback Method
vc	1.181	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.77	J/mol×K	940.17	Joback Method
cpg	942.20	J/mol×K	1122.01	Joback Method
cpg	934.65	J/mol×K	1085.65	Joback Method
cpg	925.95	J/mol×K	1049.28	Joback Method
cpg	916.08	J/mol×K	1012.91	Joback Method
cpg	905.03	J/mol×K	976.54	Joback Method
cpg	948.61	J/mol×K	1158.38	Joback Method
dvisc	0.0000375	Pa×s	940.17	Joback Method

dvisc	0.0000473	Pa×s	881.30	Joback Method
dvisc	0.0000617	Pa×s	822.43	Joback Method
dvisc	0.0000838	Pa×s	763.56	Joback Method
dvisc	0.0001199	Pa×s	704.69	Joback Method
dvisc	0.0001829	Pa×s	645.82	Joback Method
dvisc	0.0003038	Pa×s	586.95	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=U391476&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

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