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

Inchi: InChI=1S/C19H25Cl3O4/c1-2-3-4-5-6-7-11-25-17(23)9-8-10-18(24)26-19-15(21)12-14(20
InchiKey: HYOMRUHXDKVURP-UHFFFAOYSA-N
Formula: C19H25Cl3O4
SMILES: CCCCCCCCOC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]: 423.76

Physical Properties

Property code	Value	Unit	Source
gf	-311.01	kJ/mol	Joback Method
hf	-770.19	kJ/mol	Joback Method
hfus	56.00	kJ/mol	Joback Method
hvap	93.62	kJ/mol	Joback Method
log10ws	-7.31		Crippen Method
logp	6.626		Crippen Method
mcvol	306.410	ml/mol	McGowan Method
pc	1298.60	kPa	Joback Method
rinpol	2845.00		NIST Webbook
rinpol	2845.00		NIST Webbook
tb	940.61	K	Joback Method
tc	1157.50	K	Joback Method
tf	601.95	K	Joback Method
vc	1.187	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	892.29	J/mol×K	940.61	Joback Method
cpg	904.52	J/mol×K	976.76	Joback Method
cpg	915.57	J/mol×K	1012.91	Joback Method
cpg	925.46	J/mol×K	1049.06	Joback Method
cpg	934.21	J/mol×K	1085.21	Joback Method
cpg	941.84	J/mol×K	1121.35	Joback Method
cpg	948.36	J/mol×K	1157.50	Joback Method
dvisc	0.0002840	Pa×s	601.95	Joback Method

dvisc	0.0001793	Pa×s	658.39	Joback Method
dvisc	0.0001217	Pa×s	714.84	Joback Method
dvisc	0.0000874	Pa×s	771.28	Joback Method
dvisc	0.0000657	Pa×s	827.72	Joback Method
dvisc	0.0000512	Pa×s	884.17	Joback Method
dvisc	0.0000412	Pa×s	940.61	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=U358986&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