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

Inchi: InChI=1S/C18H14Cl4O4/c19-12-6-4-11(5-7-12)10-25-16(23)2-1-3-17(24)26-18-14(21)8-1

InchiKey: RODPXDOWDOTINO-UHFFFAOYSA-N

Formula: C18H14Cl4O4

SMILES: O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)OCc1ccc(Cl)cc1

Mol. weight [g/mol]: 436.11

Physical Properties

Property code	Value	Unit	Source
gf	-228.58	kJ/mol	Joback Method
hf	-540.23	kJ/mol	Joback Method
hfus	51.26	kJ/mol	Joback Method
hvap	98.71	kJ/mol	Joback Method
log10ws	-7.17		Crippen Method
logp	6.119		Crippen Method
mcvol	280.800	ml/mol	McGowan Method
pc	1736.11	kPa	Joback Method
rinpol	3098.00		NIST Webbook
rinpol	3098.00		NIST Webbook
tb	986.82	K	Joback Method
tc	1229.94	K	Joback Method
tf	659.54	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.08	J/mol×K	986.82	Joback Method
cpg	772.80	J/mol×K	1189.42	Joback Method
cpg	769.44	J/mol×K	1148.90	Joback Method
cpg	764.91	J/mol×K	1108.38	Joback Method
cpg	759.19	J/mol×K	1067.86	Joback Method
cpg	752.26	J/mol×K	1027.34	Joback Method
cpg	775.01	J/mol×K	1229.94	Joback Method
dvisc	0.0000430	Pa×s	986.82	Joback Method

dvisc	0.0000522	Pa×s	932.27	Joback Method
dvisc	0.0000650	Pa×s	877.73	Joback Method
dvisc	0.0000833	Pa×s	823.18	Joback Method
dvisc	0.0001107	Pa×s	768.63	Joback Method
dvisc	0.0001534	Pa×s	714.09	Joback Method
dvisc	0.0002246	Pa×s	659.54	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U391735&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