Glutaric acid, butyl 2,3,4,5-tetrachlorophenyl ester

Inchi: InChI=1S/C15H16Cl4O4/c1-2-3-7-22-11(20)5-4-6-12(21)23-10-8-9(16)13(17)15(19)14(10
InchiKey: GTQVTAFWWYBLAF-UHFFFAOYSA-N
Formula: C15H16Cl4O4
SMILES: CCCCOC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 402.10

Physical Properties

Property code	Value	Unit	Source
gf	-366.25	kJ/mol	Joback Method
hf	-714.84	kJ/mol	Joback Method
hfus	49.45	kJ/mol	Joback Method
hvap	89.76	kJ/mol	Joback Method
log10ws	-6.32		Crippen Method
logp	5.719		Crippen Method
mcvol	262.290	ml/mol	McGowan Method
pc	1675.53	kPa	Joback Method
rinpol	2661.00		NIST Webbook
rinpol	2661.00		NIST Webbook
tb	891.50	K	Joback Method
tc	1112.28	K	Joback Method
tf	599.31	K	Joback Method
vc	1.012	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	683.84	J/mol×K	891.50	Joback Method
cpg	693.91	J/mol×K	928.30	Joback Method
cpg	702.97	J/mol×K	965.09	Joback Method
cpg	711.02	J/mol×K	1001.89	Joback Method
cpg	718.05	J/mol×K	1038.69	Joback Method
cpg	724.08	J/mol×K	1075.49	Joback Method
cpg	729.10	J/mol×K	1112.28	Joback Method
dvisc	0.0003264	Pa×s	599.31	Joback Method

dvisc	0.0002248	Pa×s	648.01	Joback Method
dvisc	0.0001631	Pa×s	696.71	Joback Method
dvisc	0.0001234	Pa×s	745.40	Joback Method
dvisc	0.0000967	Pa×s	794.10	Joback Method
dvisc	0.0000779	Pa×s	842.80	Joback Method
dvisc	0.0000642	Pa×s	891.50	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U360749&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

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