

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

Inchi:	InChI=1S/C15H17Cl3O4/c1-2-3-7-21-13(19)5-4-6-14(20)22-15-11(17)8-10(16)9-12(15)18
InchiKey:	ZZXVPIIZFAYBIK-UHFFFAOYSA-N
Formula:	C15H17Cl3O4
SMILES:	CCCCOC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl
Mol. weight [g/mol]:	367.65

Physical Properties

Property code	Value	Unit	Source
gf	-344.69	kJ/mol	Joback Method
hf	-687.63	kJ/mol	Joback Method
hfus	45.64	kJ/mol	Joback Method
hvap	84.71	kJ/mol	Joback Method
log10ws	-5.63		Crippen Method
logp	5.066		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1749.21	kPa	Joback Method
rinqol	2433.00		NIST Webbook
tb	849.09	K	Joback Method
tc	1065.19	K	Joback Method
tf	556.87	K	Joback Method
vc	0.963	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	664.65	J/molxK	849.09	Joback Method
cpg	675.93	J/molxK	885.11	Joback Method
cpg	686.23	J/molxK	921.12	Joback Method
cpg	695.56	J/molxK	957.14	Joback Method
cpg	703.92	J/molxK	993.16	Joback Method
cpg	711.31	J/molxK	1029.18	Joback Method
cpg	717.74	J/molxK	1065.19	Joback Method
dvisc	0.0004288	Paxs	556.87	Joback Method
dvisc	0.0002840	Paxs	605.57	Joback Method

dvisc	0.0002000	Paxs	654.28	Joback Method
dvisc	0.0001478	Paxs	702.98	Joback Method
dvisc	0.0001137	Paxs	751.68	Joback Method
dvisc	0.0000902	Paxs	800.39	Joback Method
dvisc	0.0000735	Paxs	849.09	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=U358981&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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