

Glutaric acid, isobutyl 3,4,5-trichlorophenyl ester

Inchi:	InChI=1S/C15H17Cl3O4/c1-9(2)8-21-13(19)4-3-5-14(20)22-10-6-11(16)15(18)12(17)7-10
InchiKey:	XNYSESZLRODKDH-UHFFFAOYSA-N
Formula:	C15H17Cl3O4
SMILES:	CC(C)COC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)c(Cl)c1
Mol. weight [g/mol]:	367.65

Physical Properties

Property code	Value	Unit	Source
gf	-347.13	kJ/mol	Joback Method
hf	-692.91	kJ/mol	Joback Method
hfus	42.12	kJ/mol	Joback Method
hvap	84.33	kJ/mol	Joback Method
log10ws	-5.39		Crippen Method
logp	4.922		Crippen Method
mcvol	250.050	ml/mol	McGowan Method
pc	1760.97	kPa	Joback Method
rinpola	2506.00		NIST Webbook
tb	848.65	K	Joback Method
tc	1067.46	K	Joback Method
tf	541.87	K	Joback Method
vc	0.957	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	665.23	J/molxK	848.65	Joback Method
cpg	712.13	J/molxK	1030.99	Joback Method
cpg	704.76	J/molxK	994.52	Joback Method
cpg	696.40	J/molxK	958.05	Joback Method
cpg	687.02	J/molxK	921.59	Joback Method
cpg	676.64	J/molxK	885.12	Joback Method
cpg	718.50	J/molxK	1067.46	Joback Method
dvisc	0.0000674	Paxs	848.65	Joback Method
dvisc	0.0000838	Paxs	797.52	Joback Method

dvisc	0.0001074	Paxs	746.39	Joback Method
dvisc	0.0001428	Paxs	695.26	Joback Method
dvisc	0.0001987	Paxs	644.13	Joback Method
dvisc	0.0002925	Paxs	593.00	Joback Method
dvisc	0.0004634	Paxs	541.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359143&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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