

Glutaric acid, 3,5-dichlorophenyl isobutyl ester

Inchi:	InChI=1S/C15H18Cl2O4/c1-10(2)9-20-14(18)4-3-5-15(19)21-13-7-11(16)6-12(17)8-13/h
InchiKey:	SEGWAOHCFJOCTM-UHFFFAOYSA-N
Formula:	C15H18Cl2O4
SMILES:	CC(C)COC(=O)CCCC(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	333.21

Physical Properties

Property code	Value	Unit	Source
gf	-325.57	kJ/mol	Joback Method
hf	-665.70	kJ/mol	Joback Method
hfus	38.31	kJ/mol	Joback Method
hvap	79.28	kJ/mol	Joback Method
log10ws	-4.71		Crippen Method
logp	4.268		Crippen Method
mcvol	237.810	ml/mol	McGowan Method
pc	1840.41	kPa	Joback Method
rinpola	2286.00		NIST Webbook
tb	806.24	K	Joback Method
tc	1020.76	K	Joback Method
tf	499.43	K	Joback Method
vc	0.907	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	644.00	J/molxK	806.24	Joback Method
cpg	656.65	J/molxK	841.99	Joback Method
cpg	668.30	J/molxK	877.75	Joback Method
cpg	678.96	J/molxK	913.50	Joback Method
cpg	688.64	J/molxK	949.25	Joback Method
cpg	697.34	J/molxK	985.00	Joback Method
cpg	705.08	J/molxK	1020.76	Joback Method
dvisc	0.0006347	Paxs	499.43	Joback Method
dvisc	0.0003791	Paxs	550.57	Joback Method

dvisc	0.0002472	Paxs	601.70	Joback Method
dvisc	0.0001723	Paxs	652.84	Joback Method
dvisc	0.0001266	Paxs	703.97	Joback Method
dvisc	0.0000970	Paxs	755.11	Joback Method
dvisc	0.0000769	Paxs	806.24	Joback Method

Sources

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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359439&Units=SI

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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