Glutaric acid, 2,4-dichlorobenzyl isobutyl ester

Inchi: InChI=1S/C16H20Cl2O4/c1-11(2)9-21-15(19)4-3-5-16(20)22-10-12-6-7-13(17)8-14(12)18
InchiKey: XVSSANGGTOVUEO-UHFFFAOYSA-N
Formula: C16H20Cl2O4
SMILES: CC(C)COC(=O)CCCC(=O)OCc1ccc(Cl)cc1Cl
Mol. weight [g/mol]: 347.23

Physical Properties

Property code	Value	Unit	Source
gf	-317.15	kJ/mol	Joback Method
hf	-686.34	kJ/mol	Joback Method
hfus	40.90	kJ/mol	Joback Method
hvap	81.50	kJ/mol	Joback Method
log10ws	-4.97		Crippen Method
logp	4.406		Crippen Method
mcvol	251.900	ml/mol	McGowan Method
pc	1697.70	kPa	Joback Method
rinpol	2366.00		NIST Webbook
tb	829.12	K	Joback Method
tc	1042.01	K	Joback Method
tf	510.70	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.46	J/mol×K	829.12	Joback Method
cpg	753.85	J/mol×K	1006.53	Joback Method
cpg	745.00	J/mol×K	971.05	Joback Method
cpg	735.15	J/mol×K	935.56	Joback Method
cpg	724.28	J/mol×K	900.08	Joback Method
cpg	712.39	J/mol×K	864.60	Joback Method
cpg	761.71	J/mol×K	1042.01	Joback Method
dvisc	0.0000669	Pa×s	829.12	Joback Method
dvisc	0.0000847	Pa×s	776.05	Joback Method

dvisc	0.0001111	Pa×s	722.98	Joback Method
dvisc	0.0001520	Pa×s	669.91	Joback Method
dvisc	0.0002196	Pa×s	616.84	Joback Method
dvisc	0.0003401	Pa×s	563.77	Joback Method
dvisc	0.0005767	Pa×s	510.70	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U376801&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

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