Glutaric acid, butyl 2-chloro-5-methylphenyl ester

Inchi: InChI=1S/C16H21ClO4/c1-3-4-10-20-15(18)6-5-7-16(19)21-14-11-12(2)8-9-13(14)17/h8-

InchiKey: HKWDXCYJYZCQMJ-UHFFFAOYSA-N

Formula: C16H21ClO4

SMILES: CCCCOC(=O)CCCC(=O)Oc1cc(C)ccc1Cl

Mol. weight [g/mol]: 312.79

Physical Properties

Property code	Value	Unit	Source
gf	-302.78	kJ/mol	Joback Method
hf	-665.32	kJ/mol	Joback Method
hfus	40.23	kJ/mol	Joback Method
hvap	77.51	kJ/mol	Joback Method
log10ws	-4.74		Crippen Method
logp	4.067		Crippen Method
mcvol	239.660	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rinpol	2267.00		NIST Webbook
rinpol	2267.00		NIST Webbook
tb	792.13	K	Joback Method
tc	998.52	K	Joback Method
tf	495.78	K	Joback Method
vc	0.920	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	674.17	J/mol×K	792.13	Joback Method
cpg	688.09	J/mol×K	826.53	Joback Method
cpg	701.02	J/mol×K	860.93	Joback Method
cpg	712.98	J/mol×K	895.32	Joback Method
cpg	723.98	J/mol×K	929.72	Joback Method
cpg	734.02	J/mol×K	964.12	Joback Method
cpg	743.12	J/mol×K	998.52	Joback Method
dvisc	0.0006188	Pa×s	495.78	Joback Method

dvisc	0.0003809	Pa×s	545.17	Joback Method
dvisc	0.0002541	Pa×s	594.56	Joback Method
dvisc	0.0001804	Pa×s	643.96	Joback Method
dvisc	0.0001345	Pa×s	693.35	Joback Method
dvisc	0.0001042	Pa×s	742.74	Joback Method
dvisc	0.0000834	Pa×s	792.13	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=U359332&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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