Glutaric acid, monochloride, 4-bromophenyl ester

Inchi: InChI=1S/C11H10BrClO3/c12-8-4-6-9(7-5-8)16-11(15)3-1-2-10(13)14/h4-7H,1-3H2
InchiKey: AOWDQVYPNSNHTI-UHFFFAOYSA-N
Formula: C11H10BrClO3
SMILES: O=C(Cl)CCCC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 305.55

Physical Properties

Property code	Value	Unit	Source
gf	-215.93	kJ/mol	Joback Method
hf	-392.10	kJ/mol	Joback Method
hfus	31.77	kJ/mol	Joback Method
hvap	69.74	kJ/mol	Joback Method
log10ws	-4.13		Crippen Method
logp	3.290		Crippen Method
mcvol	180.840	ml/mol	McGowan Method
pc	3028.94	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook
tb	716.49	K	Joback Method
tc	948.49	K	Joback Method
tf	464.48	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	419.49	J/mol×K	716.49	Joback Method
cpg	430.07	J/mol×K	755.16	Joback Method
cpg	439.82	J/mol×K	793.82	Joback Method
cpg	448.78	J/mol×K	832.49	Joback Method
cpg	456.97	J/mol×K	871.16	Joback Method
cpg	464.43	J/mol×K	909.82	Joback Method
cpg	471.18	J/mol×K	948.49	Joback Method
dvisc	0.0010764	Pa×s	464.48	Joback Method

dvisc	0.0007014	Pa×s	506.48	Joback Method
dvisc	0.0004880	Pa×s	548.48	Joback Method
dvisc	0.0003576	Pa×s	590.49	Joback Method
dvisc	0.0002730	Pa×s	632.49	Joback Method
dvisc	0.0002156	Pa×s	674.49	Joback Method
dvisc	0.0001750	Pa×s	716.49	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U358735&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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