1,2-Cyclohexanedicarboxylic acid, 4-bromophenyl ethyl ester

Inchi: InChI=1S/C16H19BrO4/c1-2-20-15(18)13-5-3-4-6-14(13)16(19)21-12-9-7-11(17)8-10-12/

InchiKey: KKEOENSCRNNBQG-UHFFFAOYSA-N

Formula: C16H19BrO4

SMILES: CCOC(=O)C1CCCCC1C(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 355.22

Physical Properties

Property code	Value	Unit	Source
gf	-250.16	kJ/mol	Joback Method
hf	-577.80	kJ/mol	Joback Method
hfus	34.61	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Joback Method
log10ws	-4.57		Crippen Method
logp	3.724		Crippen Method
mcvol	234.060	ml/mol	McGowan Method
pc	2256.81	kPa	Joback Method
rinpol	2357.00		NIST Webbook
rinpol	2357.00		NIST Webbook
tb	830.76	K	Joback Method
tc	1069.90	K	Joback Method
tf	516.28	K	Joback Method
vc	0.866	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	684.85	J/mol×K	830.76	Joback Method
cpg	745.96	J/mol×K	1030.04	Joback Method
cpg	736.63	J/mol×K	990.18	Joback Method
cpg	725.89	J/mol×K	950.33	Joback Method
cpg	713.69	J/mol×K	910.47	Joback Method
cpg	700.02	J/mol×K	870.62	Joback Method
cpg	753.89	J/mol×K	1069.90	Joback Method
dvisc	0.0001026	Pa×s	830.76	Joback Method

dvisc	0.0001277	Pa×s	778.35	Joback Method
dvisc	0.0001640	Pa×s	725.93	Joback Method
dvisc	0.0002189	Pa×s	673.52	Joback Method
dvisc	0.0003069	Pa×s	621.11	Joback Method
dvisc	0.0004580	Pa×s	568.69	Joback Method
dvisc	0.0007412	Pa×s	516.28	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=U339624&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