Glutaric acid, cyclohexylmethyl 4-bromophenyl ester

Inchi: InChI=1S/C18H23BrO4/c19-15-9-11-16(12-10-15)23-18(21)8-4-7-17(20)22-13-14-5-2-1-3

InchiKey: AYQGJYGOZMWWGO-UHFFFAOYSA-N

Formula: C18H23BrO4

SMILES: O=C(CCCC(=O)Oc1ccc(Br)cc1)OCC1CCCCC1

Mol. weight [g/mol]: 383.28

Physical Properties

Property code	Value	Unit	Source
gf	-225.61	kJ/mol	Joback Method
hf	-598.74	kJ/mol	Joback Method
hfus	38.72	kJ/mol	Joback Method
hvap	83.78	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.648		Crippen Method
mcvol	262.240	ml/mol	McGowan Method
pc	1950.95	kPa	Joback Method
rinpol	2723.00		NIST Webbook
rinpol	2723.00		NIST Webbook
tb	881.19	K	Joback Method
tc	1113.91	K	Joback Method
tf	543.06	K	Joback Method
vc	0.979	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	794.88	J/mol×K	881.19	Joback Method
cpg	809.65	J/mol×K	919.98	Joback Method
cpg	822.97	J/mol×K	958.76	Joback Method
cpg	834.88	J/mol×K	997.55	Joback Method
cpg	845.42	J/mol×K	1036.34	Joback Method
cpg	854.64	J/mol×K	1075.12	Joback Method
cpg	862.57	J/mol×K	1113.91	Joback Method
dvisc	0.0005460	Pa×s	543.06	Joback Method

dvisc	0.0003174	Pa×s	599.41	Joback Method
dvisc	0.0002026	Pa×s	655.77	Joback Method
dvisc	0.0001388	Pa×s	712.12	Joback Method
dvisc	0.0001005	Pa×s	768.48	Joback Method
dvisc	0.0000761	Pa×s	824.83	Joback Method
dvisc	0.0000597	Pa×s	881.19	Joback Method

Sources

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=U393294&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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