Fumaric acid, 4-bromophenyl cyclohexylmethyl ester

Inchi: InChI=1S/C17H19BrO4/c18-14-6-8-15(9-7-14)22-17(20)11-10-16(19)21-12-13-4-2-1-3-5-

InchiKey: QBCQECIKBXAGHE-ZHACJKMWSA-N

Formula: C17H19BrO4

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

Mol. weight [g/mol]: 367.23

Physical Properties

Property code	Value	Unit	Source
gf	-153.81	kJ/mol	Joback Method
hf	-460.88	kJ/mol	Joback Method
hfus	36.33	kJ/mol	Joback Method
hvap	81.51	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.034		Crippen Method
mcvol	243.850	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	2582.00		NIST Webbook
rinpol	2582.00		NIST Webbook
tb	862.47	K	Joback Method
tc	1105.43	K	Joback Method
tf	526.71	K	Joback Method
vc	0.902	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.16	J/mol×K	862.47	Joback Method
cpg	724.52	J/mol×K	902.96	Joback Method
cpg	737.49	J/mol×K	943.46	Joback Method
cpg	749.14	J/mol×K	983.95	Joback Method
cpg	759.54	J/mol×K	1024.44	Joback Method
cpg	768.73	J/mol×K	1064.94	Joback Method
cpg	776.79	J/mol×K	1105.43	Joback Method
dvisc	0.0005601	Pa×s	526.71	Joback Method

dvisc	0.0003232	Pa×s	582.67	Joback Method
dvisc	0.0002054	Pa×s	638.63	Joback Method
dvisc	0.0001404	Pa×s	694.59	Joback Method
dvisc	0.0001016	Pa×s	750.55	Joback Method
dvisc	0.0000769	Pa×s	806.51	Joback Method
dvisc	0.0000603	Pa×s	862.47	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=U405773&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