

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: QBCQEICKBXAGHE-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
mvol	243.850	ml/mol	McGowan Method
pc	2233.41	kPa	Joback Method
rinpol	2582.00		NIST Webbook
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tb	862.47	K	Joback Method
tc	1105.43	K	Joback Method
tf	526.71	K	Joback Method
vc	0.902	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	710.16	J/molxK	862.47	Joback Method
cpg	768.73	J/molxK	1064.94	Joback Method
cpg	759.54	J/molxK	1024.44	Joback Method
cpg	749.14	J/molxK	983.95	Joback Method
cpg	737.49	J/molxK	943.46	Joback Method
cpg	724.52	J/molxK	902.96	Joback Method
cpg	776.79	J/molxK	1105.43	Joback Method
dvisc	0.0000603	Paxs	862.47	Joback Method

dvisc	0.0000769	Paxs	806.51	Joback Method
dvisc	0.0001016	Paxs	750.55	Joback Method
dvisc	0.0001404	Paxs	694.59	Joback Method
dvisc	0.0002054	Paxs	638.63	Joback Method
dvisc	0.0003232	Paxs	582.67	Joback Method
dvisc	0.0005601	Paxs	526.71	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

cp_g:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
g_f:	Standard Gibbs free energy of formation
h_f:	Enthalpy of formation at standard conditions
h_{fus}:	Enthalpy of fusion at standard conditions
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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