

Fumaric acid, 4-bromophenyl 2,4,6-trichlorophenyl ester

Inchi:	InChI=1S/C16H8BrCl3O4/c17-9-1-3-11(4-2-9)23-14(21)5-6-15(22)24-16-12(19)7-10(18)8
InchiKey:	DHNXVKLXNOPOQA-AATRIKPKSA-N
Formula:	C16H8BrCl3O4
SMILES:	O=C(C=CC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	450.50

Physical Properties

Property code	Value	Unit	Source
gf	-138.95	kJ/mol	Joback Method
hf	-339.66	kJ/mol	Joback Method
hfus	47.37	kJ/mol	Joback Method
hvap	96.27	kJ/mol	Joback Method
log10ws	-6.82		Crippen Method
logp	5.476		Crippen Method
mcvol	253.580	ml/mol	McGowan Method
pc	2379.54	kPa	Joback Method
rinqol	2926.00		NIST Webbook
tb	973.95	K	Joback Method
tc	1234.70	K	Joback Method
tf	661.80	K	Joback Method
vc	0.953	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	609.49	J/molxK	973.95	Joback Method
cpg	636.18	J/molxK	1191.24	Joback Method
cpg	632.57	J/molxK	1147.78	Joback Method
cpg	628.15	J/molxK	1104.32	Joback Method
cpg	622.87	J/molxK	1060.87	Joback Method
cpg	616.66	J/molxK	1017.41	Joback Method
cpg	639.04	J/molxK	1234.70	Joback Method
dvisc	0.0000458	Paxs	973.95	Joback Method
dvisc	0.0000551	Paxs	921.93	Joback Method

dvisc	0.0000677	Paxs	869.90	Joback Method
dvisc	0.0000855	Paxs	817.88	Joback Method
dvisc	0.0001115	Paxs	765.85	Joback Method
dvisc	0.0001510	Paxs	713.83	Joback Method
dvisc	0.0002146	Paxs	661.80	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=U405776&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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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