Fumaric acid, 4-bromophenyl hept-2-yl ester

Inchi: InChI=1S/C17H21BrO4/c1-3-4-5-6-13(2)21-16(19)11-12-17(20)22-15-9-7-14(18)8-10-15/
InchiKey: JHJKUUXLWREBEE-VAWYXSNFSA-N
Formula: C17H21BrO4
SMILES: CCCCCC(C)OC(=O)C=CC(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]: 369.25

Physical Properties

Property code	Value	Unit	Source
gf	-180.70	kJ/mol	Joback Method
hf	-520.48	kJ/mol	Joback Method
hfus	40.98	kJ/mol	Joback Method
hvap	80.69	kJ/mol	Joback Method
log10ws	-5.54		Crippen Method
logp	4.423		Crippen Method
mcvol	254.710	ml/mol	McGowan Method
pc	1869.17	kPa	Joback Method
rinpol	2381.00		NIST Webbook
rinpol	2381.00		NIST Webbook
tb	842.48	K	Joback Method
tc	1061.54	K	Joback Method
tf	504.33	K	Joback Method
vc	0.964	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	717.79	J/mol×K	842.48	Joback Method
cpg	731.26	J/mol×K	878.99	Joback Method
cpg	743.72	J/mol×K	915.50	Joback Method
cpg	755.20	J/mol×K	952.01	Joback Method
cpg	765.74	J/mol×K	988.52	Joback Method
cpg	775.40	J/mol×K	1025.03	Joback Method
cpg	784.21	J/mol×K	1061.54	Joback Method
dvisc	0.0005485	Pa×s	504.33	Joback Method

dvisc	0.0003060	Pa×s	560.69	Joback Method
dvisc	0.0001899	Pa×s	617.05	Joback Method
dvisc	0.0001276	Pa×s	673.40	Joback Method
dvisc	0.0000912	Pa×s	729.76	Joback Method
dvisc	0.0000684	Pa×s	786.12	Joback Method
dvisc	0.0000533	Pa×s	842.48	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405770&Units=SI
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

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