Fumaric acid, 4-bromophenyl 2-ethylhexyl ester

Inchi: InChI=1S/C18H23BrO4/c1-3-5-6-14(4-2)13-22-17(20)11-12-18(21)23-16-9-7-15(19)8-10-

InchiKey: UEDJPDQMTDLZMH-VAWYXSNFSA-N

Formula: C18H23BrO4

SMILES: CCCCC(CC)COC(=O)C=CC(=O)Oc1ccc(Br)cc1

Mol. weight [g/mol]: 383.28

Physical Properties

Property code	Value	Unit	Source
gf	-172.28	kJ/mol	Joback Method
hf	-541.12	kJ/mol	Joback Method
hfus	43.57	kJ/mol	Joback Method
hvap	82.92	kJ/mol	Joback Method
log10ws	-5.61		Crippen Method
logp	4.670		Crippen Method
mcvol	268.800	ml/mol	McGowan Method
pc	1723.16	kPa	Joback Method
rinpol	2507.00		NIST Webbook
rinpol	2507.00		NIST Webbook
tb	865.36	K	Joback Method
tc	1083.00	K	Joback Method
tf	515.60	K	Joback Method
vc	1.020	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	774.63	J/mol×K	865.36	Joback Method
cpg	788.35	J/mol×K	901.63	Joback Method
cpg	801.03	J/mol×K	937.91	Joback Method
cpg	812.72	J/mol×K	974.18	Joback Method
cpg	823.47	J/mol×K	1010.46	Joback Method
cpg	833.31	J/mol×K	1046.73	Joback Method
cpg	842.29	J/mol×K	1083.00	Joback Method
dvisc	0.0004933	Pa×s	515.60	Joback Method

dvisc	0.0002719	Pa×s	573.89	Joback Method
dvisc	0.0001673	Pa×s	632.19	Joback Method
dvisc	0.0001117	Pa×s	690.48	Joback Method
dvisc	0.0000795	Pa×s	748.77	Joback Method
dvisc	0.0000594	Pa×s	807.07	Joback Method
dvisc	0.0000461	Pa×s	865.36	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U405772&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

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