Phthalic acid, 2-(3-bromophenyl)ethyl ethyl ester

Inchi: InChI=1S/C18H17BrO4/c1-2-22-17(20)15-8-3-4-9-16(15)18(21)23-11-10-13-6-5-7-14(19)

InchiKey: HDVASJDLQFWOAC-UHFFFAOYSA-N

Formula: C18H17BrO4

SMILES: CCOC(=O)c1ccccc1C(=O)OCCc1cccc(Br)c1

Mol. weight [g/mol]: 377.23

Physical Properties

Property code	Value	Unit	Source
gf	-147.28	kJ/mol	Joback Method
hf	-428.00	kJ/mol	Joback Method
hfus	40.54	kJ/mol	Joback Method
hvap	86.28	kJ/mol	Joback Method
log10ws	-5.57		Crippen Method
logp	4.025		Crippen Method
mcvol	249.340	ml/mol	McGowan Method
pc	2157.31	kPa	Joback Method
rinpol	2593.00		NIST Webbook
tb	893.30	K	Joback Method
tc	1131.83	K	Joback Method
tf	574.62	K	Joback Method
vc	0.938	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	699.78	J/mol×K	893.30	Joback Method
cpg	711.67	J/mol×K	933.06	Joback Method
cpg	722.33	J/mol×K	972.81	Joback Method
cpg	731.82	J/mol×K	1012.57	Joback Method
cpg	740.17	J/mol×K	1052.32	Joback Method
cpg	747.42	J/mol×K	1092.08	Joback Method
cpg	753.62	J/mol×K	1131.83	Joback Method
dvisc	0.0003867	Pa×s	574.62	Joback Method
dvisc	0.0002489	Pa×s	627.73	Joback Method

dvisc	0.0001716	Pa×s	680.85	Joback Method
dvisc	0.0001249	Pa×s	733.96	Joback Method
dvisc	0.0000949	Pa×s	787.07	Joback Method
dvisc	0.0000746	Pa×s	840.19	Joback Method
dvisc	0.0000604	Pa×s	893.30	Joback Method

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U378020&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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