

Phthalic acid, 7-bromoheptyl ethyl ester

Inchi:	InChI=1S/C17H23BrO4/c1-2-21-16(19)14-10-6-7-11-15(14)17(20)22-13-9-5-3-4-8-12-18
InchiKey:	MUGGLSNBJCYIQC-UHFFFAOYSA-N
Formula:	C17H23BrO4
SMILES:	CCOC(=O)c1cccc1C(=O)OCCCCCBr
Mol. weight [g/mol]:	371.27

Physical Properties

Property code	Value	Unit	Source
gf	-258.48	kJ/mol	Joback Method
hf	-632.42	kJ/mol	Joback Method
hfus	44.30	kJ/mol	Joback Method
hvap	81.12	kJ/mol	Joback Method
log10ws	-5.32		Crippen Method
logp	4.365		Crippen Method
mvol	259.010	ml/mol	McGowan Method
pc	1775.84	kPa	Joback Method
rinpol	2675.00		NIST Webbook
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tb	838.76	K	Joback Method
tc	1049.57	K	Joback Method
tf	524.41	K	Joback Method
vc	0.990	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	744.01	J/molxK	838.76	Joback Method
cpg	757.80	J/molxK	873.90	Joback Method
cpg	770.55	J/molxK	909.03	Joback Method
cpg	782.28	J/molxK	944.17	Joback Method
cpg	793.04	J/molxK	979.30	Joback Method
cpg	802.83	J/molxK	1014.44	Joback Method
cpg	811.68	J/molxK	1049.57	Joback Method
dvisc	0.0005356	Paxs	524.41	Joback Method

dvisc	0.0003233	Paxs	576.80	Joback Method
dvisc	0.0002123	Paxs	629.19	Joback Method
dvisc	0.0001487	Paxs	681.59	Joback Method
dvisc	0.0001096	Paxs	733.98	Joback Method
dvisc	0.0000841	Paxs	786.37	Joback Method
dvisc	0.0000667	Paxs	838.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415516&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cp_g:	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:	Log ₁₀ 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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