Phthalic acid, 7-bromoheptyl hexyl ester

Inchi: InChI=1S/C21H31BrO4/c1-2-3-4-11-16-25-20(23)18-13-8-9-14-19(18)21(24)26-17-12-7-5

InchiKey: KPKSXSICYPBASH-UHFFFAOYSA-N

Formula: C21H31BrO4

SMILES: CCCCCCOC(=O)c1ccccc1C(=O)OCCCCCCCBr

Mol. weight [g/mol]: 427.37

Physical Properties

Property code	Value	Unit	Source
gf	-224.80	kJ/mol	Joback Method
hf	-714.98	kJ/mol	Joback Method
hfus	54.66	kJ/mol	Joback Method
hvap	90.02	kJ/mol	Joback Method
log10ws	-6.99		Crippen Method
logp	5.926		Crippen Method
mcvol	315.370	ml/mol	McGowan Method
pc	1315.61	kPa	Joback Method
rinpol	3065.00		NIST Webbook
rinpol	3065.00		NIST Webbook
tb	930.28	K	Joback Method
tc	1143.52	K	Joback Method
tf	569.49	K	Joback Method
vc	1.214	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	977.64	J/mol×K	930.28	Joback Method
cpg	992.30	J/mol×K	965.82	Joback Method
cpg	1005.78	J/mol×K	1001.36	Joback Method
cpg	1018.09	J/mol×K	1036.90	Joback Method
cpg	1029.29	J/mol×K	1072.44	Joback Method
cpg	1039.42	J/mol×K	1107.98	Joback Method
cpg	1048.51	J/mol×K	1143.52	Joback Method
dvisc	0.0003471	Pa×s	569.49	Joback Method

dvisc	0.0001999	Pa×s	629.62	Joback Method
dvisc	0.0001267	Pa×s	689.75	Joback Method
dvisc	0.0000864	Pa×s	749.88	Joback Method
dvisc	0.0000624	Pa×s	810.02	Joback Method
dvisc	0.0000471	Pa×s	870.15	Joback Method
dvisc	0.0000369	Pa×s	930.28	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415520&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