

Phthalic acid, 7-bromoheptyl heptyl ester

Inchi:	InChI=1S/C22H33BrO4/c1-2-3-4-7-12-17-26-21(24)19-14-9-10-15-20(19)22(25)27-18-13
InchiKey:	VMSYKPRVSOXOBS-UHFFFAOYSA-N
Formula:	C22H33BrO4
SMILES:	CCCCCCCOC(=O)c1cccc1C(=O)OCCCCCBr
Mol. weight [g/mol]:	441.40

Physical Properties

Property code	Value	Unit	Source
gf	-216.38	kJ/mol	Joback Method
hf	-735.62	kJ/mol	Joback Method
hfus	57.25	kJ/mol	Joback Method
hvap	92.25	kJ/mol	Joback Method
log10ws	-7.41		Crippen Method
logp	6.316		Crippen Method
mvol	329.460	ml/mol	McGowan Method
pc	1228.56	kPa	Joback Method
rinpol	2893.00		NIST Webbook
rinpol	2893.00		NIST Webbook
tb	953.16	K	Joback Method
tc	1169.05	K	Joback Method
tf	580.76	K	Joback Method
vc	1.270	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1037.74	J/molxK	953.16	Joback Method
cpg	1100.14	J/molxK	1133.06	Joback Method
cpg	1089.98	J/molxK	1097.08	Joback Method
cpg	1078.70	J/molxK	1061.10	Joback Method
cpg	1066.27	J/molxK	1025.12	Joback Method
cpg	1052.63	J/molxK	989.14	Joback Method
cpg	1109.23	J/molxK	1169.05	Joback Method
dvisc	0.0000317	Paxs	953.16	Joback Method

dvisc	0.0000406	Paxs	891.09	Joback Method
dvisc	0.0000539	Paxs	829.03	Joback Method
dvisc	0.0000750	Paxs	766.96	Joback Method
dvisc	0.0001106	Paxs	704.89	Joback Method
dvisc	0.0001759	Paxs	642.83	Joback Method
dvisc	0.0003088	Paxs	580.76	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U415521&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

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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