

Diethylmalonic acid, 4-bromophenyl nonyl ester

Inchi:	InChI=1S/C22H33BrO4/c1-4-7-8-9-10-11-12-17-26-20(24)22(5-2,6-3)21(25)27-19-15-13
InchiKey:	CNDMVQJNAFPGRR-UHFFFAOYSA-N
Formula:	C22H33BrO4
SMILES:	CCCCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Br)cc1
Mol. weight [g/mol]:	441.40

Physical Properties

Property code	Value	Unit	Source
gf	-213.54	kJ/mol	Joback Method
hf	-744.37	kJ/mol	Joback Method
hfus	49.83	kJ/mol	Joback Method
hvap	90.95	kJ/mol	Joback Method
log10ws	-7.43		Crippen Method
logp	6.455		Crippen Method
mvol	329.460	ml/mol	McGowan Method
pc	1245.09	kPa	Joback Method
rinpol	2671.00		NIST Webbook
rinpol	2671.00		NIST Webbook
tb	949.93	K	Joback Method
tc	1168.16	K	Joback Method
tf	583.18	K	Joback Method
vc	1.258	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1038.02	J/molxK	949.93	Joback Method
cpg	1053.00	J/molxK	986.30	Joback Method
cpg	1066.82	J/molxK	1022.67	Joback Method
cpg	1079.54	J/molxK	1059.05	Joback Method
cpg	1091.21	J/molxK	1095.42	Joback Method
cpg	1101.92	J/molxK	1131.79	Joback Method
cpg	1111.73	J/molxK	1168.16	Joback Method
dvisc	0.0002670	Paxs	583.18	Joback Method

dvisc	0.0001480	Paxs	644.31	Joback Method
dvisc	0.0000909	Paxs	705.43	Joback Method
dvisc	0.0000603	Paxs	766.56	Joback Method
dvisc	0.0000425	Paxs	827.68	Joback Method
dvisc	0.0000315	Paxs	888.80	Joback Method
dvisc	0.0000242	Paxs	949.93	Joback Method

Sources

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=U369828&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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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