

# Diethylmalonic acid, 3-bromobenzyl heptyl ester

Inchi:	InChI=1S/C21H31BrO4/c1-4-7-8-9-10-14-25-19(23)21(5-2,6-3)20(24)26-16-17-12-11-13
InchiKey:	AVAVCNXZQSJTTN-UHFFFAOYSA-N
Formula:	C21H31BrO4
SMILES:	CCCCCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(Br)c1
Mol. weight [g/mol]:	427.37

## Physical Properties

Property code	Value	Unit	Source
gf	-221.96	kJ/mol	Joback Method
hf	-723.73	kJ/mol	Joback Method
hfus	47.24	kJ/mol	Joback Method
hvap	88.73	kJ/mol	Joback Method
log10ws	-6.86		Crippen Method
logp	5.812		Crippen Method
mcvol	315.370	ml/mol	McGowan Method
pc	1333.93	kPa	Joback Method
rinpol	2535.00		NIST Webbook
rinpol	2535.00		NIST Webbook
tb	927.05	K	Joback Method
tc	1143.73	K	Joback Method
tf	571.91	K	Joback Method
vc	1.202	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	978.07	J/molxK	927.05	Joback Method
cpg	992.85	J/molxK	963.16	Joback Method
cpg	1006.49	J/molxK	999.28	Joback Method
cpg	1019.04	J/molxK	1035.39	Joback Method
cpg	1030.58	J/molxK	1071.50	Joback Method
cpg	1041.16	J/molxK	1107.62	Joback Method
cpg	1050.85	J/molxK	1143.73	Joback Method
dvisc	0.0003024	Paxs	571.91	Joback Method

dvisc	0.0001694	Paxs	631.10	Joback Method
dvisc	0.0001049	Paxs	690.29	Joback Method
dvisc	0.0000700	Paxs	749.48	Joback Method
dvisc	0.0000496	Paxs	808.67	Joback Method
dvisc	0.0000368	Paxs	867.86	Joback Method
dvisc	0.0000284	Paxs	927.05	Joback Method

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U368415&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U368415&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>

## Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>dvisc:</b>	Dynamic viscosity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</b>	Non-polar retention indices
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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