

Diethylmalonic acid, 4-bromobenzyl hexyl ester

Inchi:	InChI=1S/C20H29BrO4/c1-4-7-8-9-14-24-18(22)20(5-2,6-3)19(23)25-15-16-10-12-17(21)
InchiKey:	YEUWIWNUJWWCSS-UHFFFAOYSA-N
Formula:	C20H29BrO4
SMILES:	CCCCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(Br)cc1
Mol. weight [g/mol]:	413.35

Physical Properties

Property code	Value	Unit	Source
gf	-230.38	kJ/mol	Joback Method
hf	-703.09	kJ/mol	Joback Method
hfus	44.65	kJ/mol	Joback Method
hvap	86.50	kJ/mol	Joback Method
log10ws	-6.44		Crippen Method
logp	5.422		Crippen Method
mcvol	301.280	ml/mol	McGowan Method
pc	1432.63	kPa	Joback Method
rinpol	2461.00		NIST Webbook
rinpol	2461.00		NIST Webbook
tb	904.17	K	Joback Method
tc	1120.13	K	Joback Method
tf	560.64	K	Joback Method
vc	1.147	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	918.78	J/molxK	904.17	Joback Method
cpg	933.36	J/molxK	940.16	Joback Method
cpg	946.83	J/molxK	976.16	Joback Method
cpg	959.23	J/molxK	1012.15	Joback Method
cpg	970.63	J/molxK	1048.14	Joback Method
cpg	981.08	J/molxK	1084.14	Joback Method
cpg	990.65	J/molxK	1120.13	Joback Method
dvisc	0.0003416	Paxs	560.64	Joback Method

dvisc	0.0001935	Paxs	617.89	Joback Method
dvisc	0.0001207	Paxs	675.15	Joback Method
dvisc	0.0000811	Paxs	732.40	Joback Method
dvisc	0.0000577	Paxs	789.66	Joback Method
dvisc	0.0000430	Paxs	846.91	Joback Method
dvisc	0.0000332	Paxs	904.17	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
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=U368450&Units=SI

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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