

Diethylmalonic acid, 4-bromobenzyl propyl ester

Inchi:	InChI=1S/C17H23BrO4/c1-4-11-21-15(19)17(5-2,6-3)16(20)22-12-13-7-9-14(18)10-8-13
InchiKey:	JONCTODFYOLPHL-UHFFFAOYSA-N
Formula:	C17H23BrO4
SMILES:	CCCOC(=O)C(CC)(CC)C(=O)OCc1ccc(Br)cc1
Mol. weight [g/mol]:	371.27

Physical Properties

Property code	Value	Unit	Source
gf	-255.64	kJ/mol	Joback Method
hf	-641.17	kJ/mol	Joback Method
hfus	36.88	kJ/mol	Joback Method
hvap	79.83	kJ/mol	Joback Method
log10ws	-5.18		Crippen Method
logp	4.252		Crippen Method
mcvol	259.010	ml/mol	McGowan Method
pc	1804.63	kPa	Joback Method
rinpol	2189.00		NIST Webbook
rinpol	2189.00		NIST Webbook
tb	835.53	K	Joback Method
tc	1053.80	K	Joback Method
tf	526.83	K	Joback Method
vc	0.979	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	745.36	J/molxK	835.53	Joback Method
cpg	759.34	J/molxK	871.91	Joback Method
cpg	772.26	J/molxK	908.29	Joback Method
cpg	784.15	J/molxK	944.66	Joback Method
cpg	795.06	J/molxK	981.04	Joback Method
cpg	805.06	J/molxK	1017.42	Joback Method
cpg	814.18	J/molxK	1053.80	Joback Method
dvisc	0.0004832	Paxs	526.83	Joback Method

dvisc	0.0002836	Paxs	578.28	Joback Method
dvisc	0.0001816	Paxs	629.73	Joback Method
dvisc	0.0001244	Paxs	681.18	Joback Method
dvisc	0.0000898	Paxs	732.63	Joback Method
dvisc	0.0000677	Paxs	784.08	Joback Method
dvisc	0.0000529	Paxs	835.53	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=U368446&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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