

Diethylmalonic acid, 4-bromobenzyl isobutyl ester

Inchi:	InChI=1S/C18H25BrO4/c1-5-18(6-2,16(20)22-11-13(3)4)17(21)23-12-14-7-9-15(19)10-8
InchiKey:	ACGXGDSSMKVNNQ-UHFFFAOYSA-N
Formula:	C18H25BrO4
SMILES:	CCC(CC)(C(=O)OCc1ccc(Br)cc1)C(=O)OCC(C)C
Mol. weight [g/mol]:	385.29

Physical Properties

Property code	Value	Unit	Source
gf	-249.66	kJ/mol	Joback Method
hf	-667.09	kJ/mol	Joback Method
hfus	35.95	kJ/mol	Joback Method
hvap	81.66	kJ/mol	Joback Method
log10ws	-5.36		Crippen Method
logp	4.498		Crippen Method
mcvol	273.100	ml/mol	McGowan Method
pc	1676.91	kPa	Joback Method
rinpol	2235.00		NIST Webbook
rinpol	2235.00		NIST Webbook
tb	857.97	K	Joback Method
tc	1077.41	K	Joback Method
tf	523.10	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	802.91	J/molxK	857.97	Joback Method
cpg	817.25	J/molxK	894.54	Joback Method
cpg	830.48	J/molxK	931.12	Joback Method
cpg	842.63	J/molxK	967.69	Joback Method
cpg	853.76	J/molxK	1004.26	Joback Method
cpg	863.93	J/molxK	1040.83	Joback Method
cpg	873.19	J/molxK	1077.41	Joback Method
dvisc	0.0004828	Paxs	523.10	Joback Method

dvisc	0.0002634	Paxs	578.91	Joback Method
dvisc	0.0001599	Paxs	634.72	Joback Method
dvisc	0.0001052	Paxs	690.53	Joback Method
dvisc	0.0000737	Paxs	746.35	Joback Method
dvisc	0.0000542	Paxs	802.16	Joback Method
dvisc	0.0000415	Paxs	857.97	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U368447&Units=SI
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

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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