

Diethylmalonic acid, butyl 3-methylbenzyl ester

Inchi:	InChI=1S/C19H28O4/c1-5-8-12-22-17(20)19(6-2,7-3)18(21)23-14-16-11-9-10-15(4)13-16
InchiKey:	XNZZNQNBFPAGQW-UHFFFAOYSA-N
Formula:	C19H28O4
SMILES:	CCCCOC(=O)C(CC)(CC)C(=O)OCc1cccc(C)c1
Mol. weight [g/mol]:	320.42

Physical Properties

Property code	Value	Unit	Source
gf	-253.12	kJ/mol	Joback Method
hf	-708.78	kJ/mol	Joback Method
hfus	36.78	kJ/mol	Joback Method
hvap	77.84	kJ/mol	Joback Method
log10ws	-4.91		Crippen Method
logp	4.188		Crippen Method
mcvol	269.690	ml/mol	McGowan Method
pc	1462.37	kPa	Joback Method
rinpol	2065.00		NIST Webbook
tb	815.13	K	Joback Method
tc	1020.72	K	Joback Method
tf	489.57	K	Joback Method
vc	1.028	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	820.35	J/molxK	815.13	Joback Method
cpg	836.47	J/molxK	849.40	Joback Method
cpg	851.47	J/molxK	883.66	Joback Method
cpg	865.37	J/molxK	917.93	Joback Method
cpg	878.23	J/molxK	952.19	Joback Method
cpg	890.08	J/molxK	986.46	Joback Method
cpg	900.96	J/molxK	1020.72	Joback Method
dvisc	0.0006091	Paxs	489.57	Joback Method
dvisc	0.0003266	Paxs	543.83	Joback Method

dvisc	0.0001960	Paxs	598.09	Joback Method
dvisc	0.0001281	Paxs	652.35	Joback Method
dvisc	0.0000894	Paxs	706.61	Joback Method
dvisc	0.0000656	Paxs	760.87	Joback Method
dvisc	0.0000502	Paxs	815.13	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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=U369306&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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