

Diethylmalonic acid, 3,5-dichlorophenyl isobutyl ester

Inchi:	InChI=1S/C17H22Cl2O4/c1-5-17(6-2,15(20)22-10-11(3)4)16(21)23-14-8-12(18)7-13(19)9
InchiKey:	AOUINMMQQRRTGSG-UHFFFAOYSA-N
Formula:	C17H22Cl2O4
SMILES:	CCC(CC)(C(=O)OCC(C)C)C(=O)Oc1cc(Cl)cc(Cl)c1
Mol. weight [g/mol]:	361.26

Physical Properties

Property code	Value	Unit	Source
gf	-305.89	kJ/mol	Joback Method
hf	-715.73	kJ/mol	Joback Method
hfus	36.08	kJ/mol	Joback Method
hvap	82.43	kJ/mol	Joback Method
log10ws	-5.30		Crippen Method
logp	4.904		Crippen Method
mcvol	265.990	ml/mol	McGowan Method
pc	1594.89	kPa	Joback Method
rinpol	2120.00		NIST Webbook
rinpol	2120.00		NIST Webbook
tb	848.77	K	Joback Method
tc	1067.85	K	Joback Method
tf	524.39	K	Joback Method
vc	1.008	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	757.09	J/molxK	848.77	Joback Method
cpg	770.43	J/molxK	885.28	Joback Method
cpg	782.67	J/molxK	921.80	Joback Method
cpg	793.85	J/molxK	958.31	Joback Method
cpg	803.99	J/molxK	994.82	Joback Method
cpg	813.15	J/molxK	1031.33	Joback Method
cpg	821.36	J/molxK	1067.85	Joback Method
dvisc	0.0004714	Paxs	524.39	Joback Method

dvisc	0.0002665	Paxs	578.45	Joback Method
dvisc	0.0001661	Paxs	632.52	Joback Method
dvisc	0.0001115	Paxs	686.58	Joback Method
dvisc	0.0000794	Paxs	740.64	Joback Method
dvisc	0.0000592	Paxs	794.71	Joback Method
dvisc	0.0000458	Paxs	848.77	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370437&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

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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