Diethylmalonic acid, 2,4-dichloro-6-formylphenyl 2-methylhex-3-yl ester

Inchi: InChI=1S/C21H28Cl2O5/c1-6-9-17(13(4)5)27-19(25)21(7-2,8-3)20(26)28-18-14(12-24)10
InchiKey: RCILYYMVCXRLGZ-UHFFFAOYSA-N
Formula: C21H28Cl2O5
SMILES: CCCC(OC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)cc1C=O)C(C)C
Mol. weight [g/mol]: 431.35

Physical Properties

Property code	Value	Unit	Source
gf	-383.80	kJ/mol	Joback Method
hf	-900.62	kJ/mol	Joback Method
hfus	44.82	kJ/mol	Joback Method
hvap	98.33	kJ/mol	Joback Method
log10ws	-6.91		Crippen Method
logp	5.886		Crippen Method
mcvol	323.920	ml/mol	McGowan Method
pc	1256.59	kPa	Joback Method
rinpol	2537.00		NIST Webbook
tb	993.49	K	Joback Method
tc	1220.80	K	Joback Method
tf	608.99	K	Joback Method
vc	1.244	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	997.84	J/mol×K	993.49	Joback Method
cpg	1009.84	J/mol×K	1031.37	Joback Method
cpg	1020.58	J/mol×K	1069.26	Joback Method
cpg	1030.10	J/mol×K	1107.14	Joback Method
cpg	1038.45	J/mol×K	1145.03	Joback Method
cpg	1045.68	J/mol×K	1182.91	Joback Method
cpg	1051.84	J/mol×K	1220.80	Joback Method
dvisc	0.0002619	Pa×s	608.99	Joback Method
dvisc	0.0001456	Pa×s	673.07	Joback Method

dvisc	0.0000897	Pa×s	737.16	Joback Method
dvisc	0.0000596	Pa×s	801.24	Joback Method
dvisc	0.0000422	Pa×s	865.32	Joback Method
dvisc	0.0000313	Pa×s	929.41	Joback Method
dvisc	0.0000241	Pa×s	993.49	Joback Method

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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=U370065&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