Diethylmalonic acid, 2,4-dichloronaphth-1-yl heptyl ester

Inchi: InChI=1S/C24H30Cl2O4/c1-4-7-8-9-12-15-29-22(27)24(5-2,6-3)23(28)30-21-18-14-11-10

InchiKey: BSMWTQKPDPVFPU-UHFFFAOYSA-N

Formula: C24H30Cl2O4

SMILES: CCCCCCCOC(=O)C(CC)(CC)C(=O)Oc1c(Cl)cc(Cl)c2ccccc12

Mol. weight [g/mol]: 453.40

Physical Properties

Property code	Value	Unit	Source
gf	-147.49	kJ/mol	Joback Method
hf	-675.33	kJ/mol	Joback Method
hfus	54.36	kJ/mol	Joback Method
hvap	100.71	kJ/mol	Joback Method
log10ws	-8.60		Crippen Method
logp	7.372		Crippen Method
mcvol	345.160	ml/mol	McGowan Method
pc	1145.99	kPa	Joback Method
rinpol	3080.00		NIST Webbook
rinpol	3080.00		NIST Webbook
tb	1033.33	K	Joback Method
tc	1267.47	K	Joback Method
tf	663.50	K	Joback Method
vc	1.329	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1084.42	J/mol×K	1033.33	Joback Method
cpg	1097.77	J/mol×K	1072.35	Joback Method
cpg	1110.10	J/mol×K	1111.38	Joback Method
cpg	1121.49	J/mol×K	1150.40	Joback Method
cpg	1132.04	J/mol×K	1189.42	Joback Method
cpg	1141.85	J/mol×K	1228.45	Joback Method
cpg	1151.02	J/mol×K	1267.47	Joback Method
dvisc	0.0002378	Pa×s	663.50	Joback Method

dvisc	0.0001524	Pa×s	725.14	Joback Method
dvisc	0.0001047	Pa×s	786.78	Joback Method
dvisc	0.0000760	Pa×s	848.41	Joback Method
dvisc	0.0000576	Pa×s	910.05	Joback Method
dvisc	0.0000452	Pa×s	971.69	Joback Method
dvisc	0.0000365	Pa×s	1033.33	Joback Method

Sources

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=U370055&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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