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

Inchi: InChI=1S/C21H24Cl2O4/c1-4-7-12-26-19(24)21(5-2,6-3)20(25)27-18-15-11-9-8-10-14(15

InchiKey: AZEKHDDESQOOCD-UHFFFAOYSA-N

Formula: C21H24Cl2O4

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

Mol. weight [g/mol]: 411.32

Physical Properties

Property code	Value	Unit	Source
gf	-172.75	kJ/mol	Joback Method
hf	-613.41	kJ/mol	Joback Method
hfus	46.59	kJ/mol	Joback Method
hvap	94.03	kJ/mol	Joback Method
log10ws	-7.35		Crippen Method
logp	6.202		Crippen Method
mcvol	302.890	ml/mol	McGowan Method
pc	1406.95	kPa	Joback Method
rinpol	2786.00		NIST Webbook
rinpol	2786.00		NIST Webbook
tb	964.69	K	Joback Method
tc	1194.50	K	Joback Method
tf	629.69	K	Joback Method
vc	1.161	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	905.76	J/mol×K	964.69	Joback Method
cpg	959.31	J/mol×K	1156.20	Joback Method
cpg	950.27	J/mol×K	1117.90	Joback Method
cpg	940.47	J/mol×K	1079.60	Joback Method
cpg	929.84	J/mol×K	1041.29	Joback Method
cpg	918.30	J/mol×K	1002.99	Joback Method
cpg	967.67	J/mol×K	1194.50	Joback Method
dvisc	0.0000571	Pa×s	964.69	Joback Method

dvisc	0.0000699	Pa×s	908.86	Joback Method
dvisc	0.0000880	Pa×s	853.02	Joback Method
dvisc	0.0001143	Pa×s	797.19	Joback Method
dvisc	0.0001545	Pa×s	741.36	Joback Method
dvisc	0.0002194	Pa×s	685.52	Joback Method
dvisc	0.0003314	Pa×s	629.69	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U370051&Units=SI
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

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