Glutaric acid, 3-methylbut-2-en-1-yl 2,4-dichloro-1-naphthyl ester

Inchi: InChI=1S/C20H20Cl2O4/c1-13(2)10-11-25-18(23)8-5-9-19(24)26-20-15-7-4-3-6-14(15)16

InchiKey: GEPOIZJZTVXYPJ-UHFFFAOYSA-N

Formula: C20H20Cl2O4

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

Mol. weight [g/mol]: 395.28

Physical Properties

Property code	Value	Unit	Source
gf	-112.34	kJ/mol	Joback Method
hf	-476.59	kJ/mol	Joback Method
hfus	50.31	kJ/mol	Joback Method
hvap	93.14	kJ/mol	Joback Method
log10ws	-7.02		Crippen Method
logp	5.732		Crippen Method
mcvol	284.500	ml/mol	McGowan Method
pc	1559.81	kPa	Joback Method
rinpol	2972.00		NIST Webbook
rinpol	2972.00		NIST Webbook
tb	949.08	K	Joback Method
tc	1179.74	K	Joback Method
tf	596.96	K	Joback Method
vc	1.097	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	817.79	J/mol×K	949.08	Joback Method
cpg	829.76	J/mol×K	987.52	Joback Method
cpg	840.81	J/mol×K	1025.97	Joback Method
cpg	851.01	J/mol×K	1064.41	Joback Method
cpg	860.43	J/mol×K	1102.85	Joback Method
cpg	869.12	J/mol×K	1141.29	Joback Method
cpg	877.17	J/mol×K	1179.74	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=U392019&Units=SI

Legend

cpg:	Ideal gas heat capacity
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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