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

Inchi: InChI=1S/C21H24Cl2O4/c1-4-18(13(2)3)26-19(24)10-7-11-20(25)27-21-15-9-6-5-8-14(15

InchiKey: QAGQVDVHJQCORU-UHFFFAOYSA-N

Formula: C21H24Cl2O4

SMILES: CCC(OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12)C(C)C

Mol. weight [g/mol]: 411.32

Physical Properties

Property code	Value	Unit	Source
gf	-180.47	kJ/mol	Joback Method
hf	-615.22	kJ/mol	Joback Method
hfus	46.96	kJ/mol	Joback Method
hvap	94.55	kJ/mol	Joback Method
log10ws	-7.46		Crippen Method
logp	6.200		Crippen Method
mcvol	302.890	ml/mol	McGowan Method
pc	1403.79	kPa	Joback Method
rinpol	2942.00		NIST Webbook
rinpol	2942.00		NIST Webbook
tb	967.04	K	Joback Method
tc	1195.44	K	Joback Method
tf	597.27	K	Joback Method
vc	1.159	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	906.18	J/mol×K	967.04	Joback Method
cpg	957.28	J/mol×K	1157.38	Joback Method
cpg	949.11	J/mol×K	1119.31	Joback Method
cpg	939.97	J/mol×K	1081.24	Joback Method
cpg	929.81	J/mol×K	1043.17	Joback Method
cpg	918.56	J/mol×K	1005.11	Joback Method
cpg	964.52	J/mol×K	1195.44	Joback Method
dvisc	0.0000623	Pa×s	967.04	Joback Method

dvisc	0.0000771	Pa×s	905.41	Joback Method
dvisc	0.0000984	Pa×s	843.78	Joback Method
dvisc	0.0001305	Pa×s	782.15	Joback Method
dvisc	0.0001816	Pa×s	720.53	Joback Method
dvisc	0.0002689	Pa×s	658.90	Joback Method
dvisc	0.0004319	Pa×s	597.27	Joback Method

Sources

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=U392018&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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