Glutaric acid, 2-ethylhexyl 2,4-dichloro-1-naphthyl ester

Inchi: InChI=1S/C23H28Cl2O4/c1-3-5-9-16(4-2)15-28-21(26)12-8-13-22(27)29-23-18-11-7-6-10

InchiKey: AKTBHYLXMHSALN-UHFFFAOYSA-N

Formula: C23H28Cl2O4

SMILES: CCCCC(CC)COC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12

Mol. weight [g/mol]: 439.37

Physical Properties

Property code	Value	Unit	Source
gf	-161.19	kJ/mol	Joback Method
hf	-651.22	kJ/mol	Joback Method
hfus	55.66	kJ/mol	Joback Method
hvap	99.39	kJ/mol	Joback Method
log10ws	-8.19		Crippen Method
logp	6.982		Crippen Method
mcvol	331.070	ml/mol	McGowan Method
pc	1214.90	kPa	Joback Method
rinpol	3186.00		NIST Webbook
rinpol	3186.00		NIST Webbook
tb	1013.24	K	Joback Method
tc	1243.38	K	Joback Method
tf	634.81	K	Joback Method
vc	1.278	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1024.30	J/mol×K	1013.24	Joback Method
cpg	1037.07	J/mol×K	1051.60	Joback Method
cpg	1048.67	J/mol×K	1089.95	Joback Method
cpg	1059.16	J/mol×K	1128.31	Joback Method
cpg	1068.61	J/mol×K	1166.67	Joback Method
cpg	1077.07	J/mol×K	1205.03	Joback Method
cpg	1084.62	J/mol×K	1243.38	Joback Method
dvisc	0.0003329	Pa×s	634.81	Joback Method

dvisc	0.0002118	Pa×s	697.88	Joback Method
dvisc	0.0001453	Pa×s	760.95	Joback Method
dvisc	0.0001055	Pa×s	824.03	Joback Method
dvisc	0.0000803	Pa×s	887.10	Joback Method
dvisc	0.0000633	Pa×s	950.17	Joback Method
dvisc	0.0000514	Pa×s	1013.24	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U392024&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

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

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