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

Inchi: InChI=1S/C21H20Cl2O4/c1-3-8-14(4-2)26-19(24)11-7-12-20(25)27-21-16-10-6-5-9-15(16

InchiKey: IIYMHMDRLUHDOB-UHFFFAOYSA-N

Formula: C21H20Cl2O4

SMILES: CC#CC(CC)OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12

Mol. weight [g/mol]: 407.29

Physical Properties

Property code	Value	Unit	Source
gf	24.77	kJ/mol	Joback Method
hf	-337.64	kJ/mol	Joback Method
hfus	53.61	kJ/mol	Joback Method
hvap	97.09	kJ/mol	Joback Method
log10ws	-7.50		Crippen Method
logp	5.567		Crippen Method
mcvol	294.290	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinpol	3009.00		NIST Webbook
rinpol	3009.00		NIST Webbook
tb	976.48	K	Joback Method
tc	1215.23	K	Joback Method
tf	718.37	K	Joback Method
vc	1.127	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	848.34	J/mol×K	976.48	Joback Method
cpg	859.89	J/mol×K	1016.27	Joback Method
cpg	870.32	J/mol×K	1056.06	Joback Method
cpg	879.68	J/mol×K	1095.85	Joback Method
cpg	888.04	J/mol×K	1135.65	Joback Method
cpg	895.43	J/mol×K	1175.44	Joback Method
cpg	901.92	J/mol×K	1215.23	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=U392021&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
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