

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

Inchi:	InChI=1S/C19H16Cl2O4/c1-3-12(2)24-17(22)9-6-10-18(23)25-19-14-8-5-4-7-13(14)15(20)
InchiKey:	QYVFIPFHMQMJOJ-UHFFFAOYSA-N
Formula:	C19H16Cl2O4
SMILES:	<chem>C#CC(C)OC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)c2ccccc12</chem>
Mol. weight [g/mol]:	379.23

Physical Properties

Property code	Value	Unit	Source
gf	28.20	kJ/mol	Joback Method
hf	-276.76	kJ/mol	Joback Method
hfus	48.28	kJ/mol	Joback Method
hvap	90.34	kJ/mol	Joback Method
log10ws	-6.66		Crippen Method
logp	4.787		Crippen Method
mvol	266.110	ml/mol	McGowan Method
pc	1830.98	kPa	Joback Method
rinpol	2763.00		NIST Webbook
rinpol	2763.00		NIST Webbook
tb	911.84	K	Joback Method
tc	1146.90	K	Joback Method
tf	636.70	K	Joback Method
vc	1.016	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	731.88	J/molxK	911.84	Joback Method
cpg	743.00	J/molxK	951.02	Joback Method
cpg	753.16	J/molxK	990.19	Joback Method
cpg	762.41	J/molxK	1029.37	Joback Method
cpg	770.81	J/molxK	1068.54	Joback Method
cpg	778.40	J/molxK	1107.72	Joback Method
cpg	785.25	J/molxK	1146.90	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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=U392016&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
hvp:	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
rinp:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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