

Glutaric acid, but-3-yn-2-yl (2-naphthyl)methyl ester

Inchi:	InChI=1S/C20H20O4/c1-3-15(2)24-20(22)10-6-9-19(21)23-14-16-11-12-17-7-4-5-8-18(17)
InchiKey:	PHAOINMHXNPYQP-UHFFFAOYSA-N
Formula:	C20H20O4
SMILES:	<chem>C#CC(C)OC(=O)CCCC(=O)OCc1ccc2ccccc2c1</chem>
Mol. weight [g/mol]:	324.37

Physical Properties

Property code	Value	Unit	Source
gf	79.74	kJ/mol	Joback Method
hf	-242.98	kJ/mol	Joback Method
hfus	43.25	kJ/mol	Joback Method
hvap	82.47	kJ/mol	Joback Method
log10ws	-5.55		Crippen Method
logp	3.618		Crippen Method
mvol	255.720	ml/mol	McGowan Method
pc	1843.58	kPa	Joback Method
rinpol	2576.00		NIST Webbook
rinpol	2576.00		NIST Webbook
tb	849.90	K	Joback Method
tc	1074.97	K	Joback Method
tf	563.09	K	Joback Method
vc	0.974	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	747.37	J/mol×K	849.90	Joback Method
cpg	761.22	J/mol×K	887.41	Joback Method
cpg	774.01	J/mol×K	924.92	Joback Method
cpg	785.81	J/mol×K	962.43	Joback Method
cpg	796.68	J/mol×K	999.95	Joback Method
cpg	806.68	J/mol×K	1037.46	Joback Method
cpg	815.87	J/mol×K	1074.97	Joback Method

Sources

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=U392195&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

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

Latest version available from:

<https://www.chemeo.com/cid/87-376-9/Glutaric-acid-but-3-yn-2-yl-2-naphthyl-methyl-ester.pdf>

Generated by Cheméo on 2024-05-05 07:59:21.886585805 +0000 UTC m=+17185210.807163116.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.