

Glutaric acid, 3-methylbut-2-en-1-yl 1-naphthyl ester

Inchi:	InChI=1S/C20H22O4/c1-15(2)13-14-23-19(21)11-6-12-20(22)24-18-10-5-8-16-7-3-4-9-17
InchiKey:	UKJAAQDOLBDUKV-UHFFFAOYSA-N
Formula:	C20H22O4
SMILES:	CC(C)=CCOC(=O)CCCC(=O)Oc1cccc2ccccc12
Mol. weight [g/mol]:	326.39

Physical Properties

Property code	Value	Unit	Source
gf	-69.22	kJ/mol	Joback Method
hf	-422.17	kJ/mol	Joback Method
hfus	42.69	kJ/mol	Joback Method
hvap	83.04	kJ/mol	Joback Method
log10ws	-5.65		Crippen Method
logp	4.425		Crippen Method
mvol	260.020	ml/mol	McGowan Method
pc	1696.30	kPa	Joback Method
rinpol	2680.00		NIST Webbook
rinpol	2680.00		NIST Webbook
tb	864.26	K	Joback Method
tc	1085.74	K	Joback Method
tf	512.08	K	Joback Method
vc	0.999	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	775.35	J/mol×K	864.26	Joback Method
cpg	789.60	J/mol×K	901.17	Joback Method
cpg	802.84	J/mol×K	938.09	Joback Method
cpg	815.15	J/mol×K	975.00	Joback Method
cpg	826.58	J/mol×K	1011.91	Joback Method
cpg	837.22	J/mol×K	1048.82	Joback Method
cpg	847.12	J/mol×K	1085.74	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393331&Units=SI
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

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
rlnol:	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.cheméo.com/cid/87-415-5/Glutaric-acid-3-methylbut-2-en-1-yl-1-naphthyl-ester.pdf>

Generated by Cheméo on 2024-05-03 18:04:48.371135749 +0000 UTC m=+17048737.291713069.

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