

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

Inchi:	InChI=1S/C20H30O4/c1-14(2)10-11-23-18(21)6-5-7-19(22)24-13-15-8-9-16-12-17(15)20
InchiKey:	FBIYGECHKBFKQA-UHFFFAOYSA-N
Formula:	C20H30O4
SMILES:	CC(C)=CCOC(=O)CCCC(=O)OCC1=CCC2CC1C2(C)C
Mol. weight [g/mol]:	334.45

Physical Properties

Property code	Value	Unit	Source
gf	-162.12	kJ/mol	Joback Method
hf	-657.65	kJ/mol	Joback Method
hfus	41.80	kJ/mol	Joback Method
hvap	77.96	kJ/mol	Joback Method
log10ws	-4.69		Crippen Method
logp	4.202		Crippen Method
mcvol	277.220	ml/mol	McGowan Method
pc	1401.69	kPa	Joback Method
rinpol	2318.00		NIST Webbook
rinpol	2318.00		NIST Webbook
tb	831.08	K	Joback Method
tc	1037.74	K	Joback Method
tf	505.74	K	Joback Method
vc	1.073	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	886.60	J/mol×K	831.08	Joback Method
cpg	905.60	J/mol×K	865.52	Joback Method
cpg	924.10	J/mol×K	899.97	Joback Method
cpg	942.22	J/mol×K	934.41	Joback Method
cpg	960.13	J/mol×K	968.85	Joback Method
cpg	977.94	J/mol×K	1003.30	Joback Method
cpg	995.81	J/mol×K	1037.74	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=U405540&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.cheméo.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
rinpola:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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