

Glutaric acid, decyl 3-methylbut-2-enyl ester

Inchi: InChI=1S/C20H36O4/c1-4-5-6-7-8-9-10-11-16-23-19(21)13-12-14-20(22)24-17-15-18(2)3
InchiKey: WVOKBBJAWPUPPI-UHFFFAOYSA-N
Formula: C20H36O4
SMILES: CCCCCCCCCCOC(=O)CCCC(=O)OCC=C(C)C
Mol. weight [g/mol]: 340.50

Physical Properties

Property code	Value	Unit	Source
gf	-278.65	kJ/mol	Joback Method
hf	-838.30	kJ/mol	Joback Method
hfus	52.02	kJ/mol	Joback Method
hvap	78.46	kJ/mol	Joback Method
log10ws	-5.77		Crippen Method
logp	5.350		Crippen Method
mvol	303.240	ml/mol	McGowan Method
pc	1119.30	kPa	Joback Method
rinpol	2412.00		NIST Webbook
rinpol	2412.00		NIST Webbook
tb	813.62	K	Joback Method
tc	1000.55	K	Joback Method
tf	440.44	K	Joback Method
vc	1.185	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	943.49	J/mol×K	813.62	Joback Method
cpg	961.24	J/mol×K	844.78	Joback Method
cpg	978.00	J/mol×K	875.93	Joback Method
cpg	993.78	J/mol×K	907.09	Joback Method
cpg	1008.61	J/mol×K	938.24	Joback Method
cpg	1022.53	J/mol×K	969.40	Joback Method
cpg	1035.56	J/mol×K	1000.55	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=U360094&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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