

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

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C14H24O4/c1-4-5-10-17-13(15)7-6-8-14(16)18-11-9-12(2)3/h9H,4-8,10-11H2,

UPGALRQSYPYJKH-UHFFFAOYSA-N

C14H24O4

CCCCOC(=O)CCCC(=O)OCC=C(C)C

256.34

Physical Properties

Property code	Value	Unit	Source
gf	-329.17	kJ/mol	Joback Method
hf	-714.46	kJ/mol	Joback Method
hfus	36.48	kJ/mol	Joback Method
hvap	65.11	kJ/mol	Joback Method
log10ws	-3.26		Crippen Method
logp	3.009		Crippen Method
mcvol	218.700	ml/mol	McGowan Method
pc	1717.45	kPa	Joback Method
rinpol	1809.00		NIST Webbook
tb	676.34	K	Joback Method
tc	859.79	K	Joback Method
tf	372.82	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	599.82	J/mol×K	676.34	Joback Method
cpg	615.14	J/mol×K	706.91	Joback Method
cpg	629.70	J/mol×K	737.49	Joback Method
cpg	643.53	J/mol×K	768.06	Joback Method
cpg	656.63	J/mol×K	798.64	Joback Method
cpg	669.02	J/mol×K	829.21	Joback Method
cpg	680.72	J/mol×K	859.79	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=U360087&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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