

Glutaric acid, neopentyl propyl ester

Inchi:	InChI=1S/C13H24O4/c1-5-9-16-11(14)7-6-8-12(15)17-10-13(2,3)4/h5-10H2,1-4H3
InchiKey:	RNQGJRYMZIWLFN-UHFFFAOYSA-N
Formula:	C13H24O4
SMILES:	CCCOC(=O)CCCC(=O)OCC(C)(C)C
Mol. weight [g/mol]:	244.33

Physical Properties

Property code	Value	Unit	Source
gf	-406.42	kJ/mol	Joback Method
hf	-810.00	kJ/mol	Joback Method
hfus	27.59	kJ/mol	Joback Method
hvap	61.55	kJ/mol	Joback Method
log10ws	-2.75		Crippen Method
logp	2.699		Crippen Method
mcvol	208.910	ml/mol	McGowan Method
pc	1803.09	kPa	Joback Method
rinqol	1577.00		NIST Webbook
tb	646.19	K	Joback Method
tc	830.33	K	Joback Method
tf	383.01	K	Joback Method
vc	0.800	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	571.18	J/molxK	646.19	Joback Method
cpg	586.81	J/molxK	676.88	Joback Method
cpg	601.65	J/molxK	707.57	Joback Method
cpg	615.71	J/molxK	738.26	Joback Method
cpg	629.03	J/molxK	768.95	Joback Method
cpg	641.60	J/molxK	799.64	Joback Method
cpg	653.44	J/molxK	830.33	Joback Method
dvisc	0.0016936	Paxs	383.01	Joback Method
dvisc	0.0008633	Paxs	426.87	Joback Method

dvisc	0.0004990	Paxs	470.74	Joback Method
dvisc	0.0003166	Paxs	514.60	Joback Method
dvisc	0.0002158	Paxs	558.46	Joback Method
dvisc	0.0001555	Paxs	602.33	Joback Method
dvisc	0.0001172	Paxs	646.19	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=U358340&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
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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