

Glutaric acid, heptyl trans-hex-3-enyl ester

Inchi:	InChI=1S/C18H32O4/c1-3-5-7-9-11-16-22-18(20)14-12-13-17(19)21-15-10-8-6-4-2/h6,8H
InchiKey:	YRGPTAVLLFYUTH-SOFGYWHQSA-N
Formula:	C18H32O4
SMILES:	CCC=CCCOC(=O)CCCC(=O)OCCCCCCC
Mol. weight [g/mol]:	312.44

Physical Properties

Property code	Value	Unit	Source
gf	-286.94	kJ/mol	Joback Method
hf	-787.23	kJ/mol	Joback Method
hfus	48.15	kJ/mol	Joback Method
hvap	73.93	kJ/mol	Joback Method
log10ws	-4.94		Crippen Method
logp	4.570		Crippen Method
mcvol	275.060	ml/mol	McGowan Method
pc	1273.69	kPa	Joback Method
rinpol	2182.00		NIST Webbook
tb	767.98	K	Joback Method
tc	950.09	K	Joback Method
tf	431.86	K	Joback Method
vc	1.071	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	825.20	J/mol×K	767.98	Joback Method
cpg	900.81	J/mol×K	919.74	Joback Method
cpg	887.40	J/mol×K	889.39	Joback Method
cpg	873.15	J/mol×K	859.03	Joback Method
cpg	858.05	J/mol×K	828.68	Joback Method
cpg	842.07	J/mol×K	798.33	Joback Method
cpg	913.41	J/mol×K	950.09	Joback Method
dvisc	0.0000613	Pa×s	767.98	Joback Method
dvisc	0.0000809	Pa×s	711.96	Joback Method

dvisc	0.0001121	Pa×s	655.94	Joback Method
dvisc	0.0001651	Pa×s	599.92	Joback Method
dvisc	0.0002633	Pa×s	543.90	Joback Method
dvisc	0.0004674	Pa×s	487.88	Joback Method
dvisc	0.0009629	Pa×s	431.86	Joback Method

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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=U359927&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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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