

Glutaric acid, hexa-1,5-dien-3-yl 2-ethylhexyl ester

Inchi:	InChI=1S/C19H32O4/c1-5-9-12-16(7-3)15-22-18(20)13-10-14-19(21)23-17(8-4)11-6-2/h6
InchiKey:	SEKOAFIU VATNAW-UHFFFAOYSA-N
Formula:	C19H32O4
SMILES:	<chem>C=CCC(C=C)OC(=O)CCCC(=O)OCC(CC)CCCC</chem>
Mol. weight [g/mol]:	324.45

Physical Properties

Property code	Value	Unit	Source
gf	-187.94	kJ/mol	Joback Method
hf	-684.79	kJ/mol	Joback Method
hfus	40.93	kJ/mol	Joback Method
hvap	74.08	kJ/mol	Joback Method
log10ws	-5.08		Crippen Method
logp	4.590		Crippen Method
mvol	284.850	ml/mol	McGowan Method
pc	1231.15	kPa	Joback Method
rinpol	2032.00		NIST Webbook
rinpol	2032.00		NIST Webbook
tb	779.18	K	Joback Method
tc	964.23	K	Joback Method
tf	414.69	K	Joback Method
vc	1.097	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	857.28	J/molxK	779.18	Joback Method
cpg	874.30	J/molxK	810.02	Joback Method
cpg	890.36	J/molxK	840.86	Joback Method
cpg	905.47	J/molxK	871.71	Joback Method
cpg	919.66	J/molxK	902.55	Joback Method
cpg	932.94	J/molxK	933.39	Joback Method
cpg	945.34	J/molxK	964.23	Joback Method
dvisc	0.0013580	Paxs	414.69	Joback Method

dvisc	0.0005764	Paxs	475.44	Joback Method
dvisc	0.0002971	Paxs	536.19	Joback Method
dvisc	0.0001752	Paxs	596.93	Joback Method
dvisc	0.0001139	Paxs	657.68	Joback Method
dvisc	0.0000797	Paxs	718.43	Joback Method
dvisc	0.0000589	Paxs	779.18	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=U405281&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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