di-(2-Ethylbutyl)glutarate

Other names: di-(2-Ethylbutyl)glutarate
Inchi: InChI=1S/C17H32O4/c1-5-14(6-2)12-20-16(18)10-9-11-17(19)21-13-15(7-3)8-4/h14-15H
InchiKey: UEQHWVKBOSUYDU-UHFFFAOYSA-N
Formula: C17H32O4
SMILES: CCC(CC)COC(=O)CCCC(=O)OCC(CC)CC
Mol. weight [g/mol]: 300.44

Physical Properties

Property code	Value	Unit	Source
hf	-1055.43	kJ/mol	Cheméo Relay (1.0)
hfus	38.31	kJ/mol	Joback Method
hvap	86.22	kJ/mol	Cheméo Relay (1.0)
ie	9.44	eV	Cheméo Relay (1.0)
log10ws	-4.13		Cheméo Relay (1.0)
logp	4.115		Crippen Method
mcvol	265.270	ml/mol	McGowan Method
pc	1330.04	kPa	Joback Method
rinpol	1925.00		NIST Webbook
rinpol	2025.00		NIST Webbook
tb	593.69	K	Cheméo Relay (1.0)
tc	754.55	K	Cheméo Relay (1.0)
tf	208.54	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	792.00	J/mol×K	740.06	Joback Method
cpg	809.35	J/mol×K	770.15	Joback Method
cpg	825.78	J/mol×K	800.24	Joback Method
cpg	841.31	J/mol×K	830.32	Joback Method
cpg	855.95	J/mol×K	860.41	Joback Method
cpg	869.70	J/mol×K	890.50	Joback Method
cpg	882.59	J/mol×K	920.59	Joback Method
dvisc	0.0016971	Pa×s	395.67	Joback Method

dvisc	0.0007096	Pa×s	453.07	Joback Method
dvisc	0.0003610	Pa×s	510.47	Joback Method
dvisc	0.0002105	Pa×s	567.87	Joback Method
dvisc	0.0001355	Pa×s	625.26	Joback Method
dvisc	0.0000940	Pa×s	682.66	Joback Method
dvisc	0.0000690	Pa×s	740.06	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U359435&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

Legend

cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
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