

Glutaric acid, but-3-en-2-yl 2-methylpent-3-yl ester

Inchi:	InChI=1S/C15H26O4/c1-6-12(5)18-14(16)9-8-10-15(17)19-13(7-2)11(3)4/h6,11-13H,1,7-
InchiKey:	UGAISORUMRFOBU-UHFFFAOYSA-N
Formula:	C15H26O4
SMILES:	C=CC(C)OC(=O)CCCC(=O)OC(CC)C(C)C
Mol. weight [g/mol]:	270.36

Physical Properties

Property code	Value	Unit	Source
gf	-311.90	kJ/mol	Joback Method
hf	-732.94	kJ/mol	Joback Method
hfus	28.33	kJ/mol	Joback Method
hvap	65.46	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.252		Crippen Method
mcvol	232.790	ml/mol	McGowan Method
pc	1600.00	kPa	Joback Method
rinpola	1633.00		NIST Webbook
tb	690.54	K	Joback Method
tc	875.49	K	Joback Method
tf	356.37	K	Joback Method
vc	0.886	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	654.81	J/molxK	690.54	Joback Method
cpg	671.12	J/molxK	721.36	Joback Method
cpg	686.58	J/molxK	752.19	Joback Method
cpg	701.21	J/molxK	783.01	Joback Method
cpg	715.01	J/molxK	813.84	Joback Method
cpg	727.99	J/molxK	844.66	Joback Method
cpg	740.16	J/molxK	875.49	Joback Method
dvisc	0.0026600	Paxs	356.37	Joback Method
dvisc	0.0010276	Paxs	412.06	Joback Method

dvisc	0.0004979	Paxs	467.76	Joback Method
dvisc	0.0002815	Paxs	523.45	Joback Method
dvisc	0.0001776	Paxs	579.15	Joback Method
dvisc	0.0001214	Paxs	634.85	Joback Method
dvisc	0.0000883	Paxs	690.54	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=U405233&Units=SI

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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