

Diallyl glutarate

Inchi:	InChI=1S/C11H16O4/c1-3-8-14-10(12)6-5-7-11(13)15-9-4-2/h3-4H,1-2,5-9H2
InchiKey:	ASDNCENZKQFYSF-UHFFFAOYSA-N
Formula:	C11H16O4
SMILES:	C=CCOC(=O)CCCC(=O)OCC=C
Mol. weight [g/mol]:	212.24

Physical Properties

Property code	Value	Unit	Source
gf	-250.42	kJ/mol	Joback Method
hf	-509.11	kJ/mol	Joback Method
hfus	27.26	kJ/mol	Joback Method
hvap	57.05	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.615		Crippen Method
mcvol	172.130	ml/mol	McGowan Method
pc	2271.90	kPa	Joback Method
rinqol	1405.00		NIST Webbook
tb	597.02	K	Joback Method
tc	781.54	K	Joback Method
tf	354.53	K	Joback Method
vc	0.661	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	423.04	J/molxK	597.02	Joback Method
cpg	435.78	J/molxK	627.77	Joback Method
cpg	447.94	J/molxK	658.53	Joback Method
cpg	459.51	J/molxK	689.28	Joback Method
cpg	470.51	J/molxK	720.03	Joback Method
cpg	480.94	J/molxK	750.78	Joback Method
cpg	490.79	J/molxK	781.54	Joback Method
dvisc	0.0017188	Paxs	354.53	Joback Method
dvisc	0.0009783	Paxs	394.94	Joback Method

dvisc	0.0006183	Paxs	435.36	Joback Method
dvisc	0.0004224	Paxs	475.77	Joback Method
dvisc	0.0003063	Paxs	516.19	Joback Method
dvisc	0.0002328	Paxs	556.61	Joback Method
dvisc	0.0001836	Paxs	597.02	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=R542302&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
mccvol:	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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