Deca-4,6-diyn-1-yl 3-methylbutanoate

Inchi: InChI=1S/C15H22O2/c1-4-5-6-7-8-9-10-11-12-17-15(16)13-14(2)3/h14H,4-5,10-13H2,1-3
InchiKey: NVMLEKVHEUTCIU-UHFFFAOYSA-N
Formula: C15H22O2
SMILES: CCCC#CC#CCCCOC(=O)CC(C)C
Mol. weight [g/mol]: 234.33
CAS: 29314-16-7

Physical Properties

Property code	Value	Unit	Source
gf	244.66	kJ/mol	Joback Method
hf	-58.41	kJ/mol	Joback Method
hfus	40.11	kJ/mol	Joback Method
hvap	62.06	kJ/mol	Joback Method
log10ws	-4.31		Crippen Method
logp	3.163		Crippen Method
mcvol	212.450	ml/mol	McGowan Method
pc	1916.94	kPa	Joback Method
rinpol	1817.40		NIST Webbook
rinpol	1773.00		NIST Webbook
rinpol	1817.40		NIST Webbook
rinpol	1773.00		NIST Webbook
ripol	2406.00		NIST Webbook
ripol	2406.00		NIST Webbook
tb	636.45	K	Joback Method
tc	842.42	K	Joback Method
tf	528.17	K	Joback Method
vc	0.818	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	540.67	J/mol×K	636.45	Joback Method
cpg	557.59	J/mol×K	670.78	Joback Method
cpg	573.66	J/mol×K	705.11	Joback Method

cpg	588.89	J/mol×K	739.44	Joback Method
cpg	603.32	J/mol×K	773.76	Joback Method
cpg	616.94	J/mol×K	808.09	Joback Method
cpg	629.77	J/mol×K	842.42	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29314167&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

cpg:	Ideal gas heat capacity
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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume