trans-3-Heptenyl butanoate

Inchi: InChI=1S/C11H20O2/c1-3-5-6-7-8-10-13-11(12)9-4-2/h6-7H,3-5,8-10H2,1-2H3/b7-6+
InchiKey: VFCAZKLWGOHHID-VOTSOKGWSA-N
Formula: C11H20O2
SMILES: CCCC=CCCOC(=O)CCC
Mol. weight [g/mol]: 184.28

Physical Properties

Property code	Value	Unit	Source
gf	-111.96	kJ/mol	Joback Method
hf	-397.95	kJ/mol	Joback Method
hfus	27.24	kJ/mol	Joback Method
hvap	49.19	kJ/mol	Joback Method
log10ws	-3.14		Crippen Method
logp	3.076		Crippen Method
mcvol	168.990	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
rinpol	1275.00		NIST Webbook
rinpol	1275.00		NIST Webbook
ripol	1568.00		NIST Webbook
ripol	1568.00		NIST Webbook
tb	531.53	K	Joback Method
tc	709.61	K	Joback Method
tf	280.81	K	Joback Method
vc	0.655	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	397.35	J/mol×K	531.53	Joback Method
cpg	464.33	J/mol×K	679.93	Joback Method
cpg	452.12	J/mol×K	650.25	Joback Method
cpg	439.33	J/mol×K	620.57	Joback Method
cpg	425.95	J/mol×K	590.89	Joback Method
cpg	411.96	J/mol×K	561.21	Joback Method

cpg	475.98	J/mol×K	709.61	Joback Method
dvisc	0.0001740	Pa×s	531.53	Joback Method
dvisc	0.0002282	Pa×s	489.74	Joback Method
dvisc	0.0003149	Pa×s	447.96	Joback Method
dvisc	0.0004643	Pa×s	406.17	Joback Method
dvisc	0.0007484	Pa×s	364.38	Joback Method
dvisc	0.0013650	Pa×s	322.60	Joback Method
dvisc	0.0029775	Pa×s	280.81	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R410309&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
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
ripol: Polar retention indices
tb: Normal Boiling Point Temperature
tc: Critical Temperature
tf: Normal melting (fusion) point
vc: Critical Volume